Access DB# _____

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: Natalie Davis Examiner #: 78462 Date: 1-8-01
Art Unit: 1642 Phone Number 308-6410 Serial Number: 09/449,763
Mail Box and Bldg/Room Location: CM1 4c01 Results Format Preferred (circle): PAPER DISK E-MAIL
8001

If more than one search is submitted, please prioritize searches in order of need.

****

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: Diagnostic Agents and Remedies for Malignant Tumors

Inventors (please provide full names): Tohru Tanaka and Hiroshi Sasaki

Earliest Priority Filing Date: 6-18-97

***For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.**

Please search 5-aminolevulic acid which may be an ester, amide, salt, hydrate or solvate and contains a carbon and/or nitrogen isotope.

BEST AVAILABLE COPY

Point of Contact:
Barb O'Bryen
Technical Info. Specialist
CM1 [illegible] Tel: 308-4291

****

STAFF USE ONLY	Type of Search		Vendors and cost where applicable	
Searcher:	BOB	NA Sequence (#)	STN	2 CA
Searcher Phone #:		AA Sequence (#)	Dialog	
Searcher Location:		Structure (#)	4	Questel/Orbit
Date Searcher Picked Up:		Bibliographic		Dr.Link
Date Completed:	1-16-01	Litigation		Lexis/Nexis
Searcher Prep & Review Time:	28	Fulltext		Sequence Systems
Clerical Prep Time:		Patent Family		WWW/Internet
Online Time:	15	Other		Other (specify)

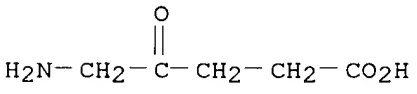
PTO-1590 (1-2000)

```
=> fil lreg; d ide l1

FILE 'LREGISTRY' ENTERED AT 16:34:07 ON 16 JAN 2001
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2001 AMERICAN CHEMICAL SOCIETY (ACS)

LREGISTRY IS A STATIC LEARNING FILE


L1   ANSWER 1 OF 1  COPYRIGHT 2001 ACS
RN   106-60-5  LREGISTRY
CN   Pentanoic acid, 5-amino-4-oxo- (9CI)  (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN   Levulinic acid, 5-amino- (8CI)
OTHER NAMES:
CN   .delta.-Aminolevulinic acid
CN   5-Aminolevulinic acid
CN   Aminolevulinic acid
FS   3D CONCORD
MF   C5 H9 N O3
CI   COM
LC   STN Files:   ADISINSIGHT, AGRICOLA, AIDSLINE, ANABSTR, BEILSTEIN*,
       BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CABA, CANCERLIT, CAOLD, CAPLUS,
       CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSNB, DDFU,
       DIOGENES, DRUGU, EMBASE, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*,
       NAPRALERT, NIOSHTIC, PHAR, PIRA, PROMT, TOXLINE, TOXLIT, USPATFULL
         (*File contains numerically searchable property data)
     Other Sources:   EINECS**, NDSL**, TSCA**
         (**Enter CHEMLIST File for up-to-date regulatory information)
```



structure of 5-aminolevulinic acid

=> fil reg; d stat que l15; fil capl; d que nos l16

FILE 'REGISTRY' ENTERED AT 16:44:13 ON 16 JAN 2001
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

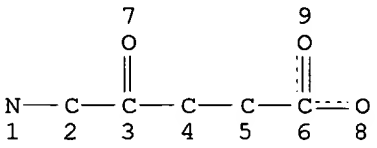
STRUCTURE FILE UPDATES: 15 JAN 2001 HIGHEST RN 314018-37-6
DICTIONARY FILE UPDATES: 15 JAN 2001 HIGHEST RN 314018-37-6

TSCA INFORMATION NOW CURRENT THROUGH July 8, 2000

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Structure search limits have been increased. See HELP SLIMIT for details.

L3 STR



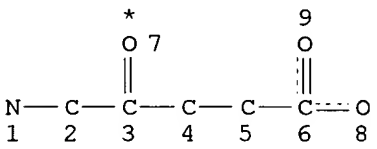
all hydrogens removed from structure to allow for esters, amides, etc

NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

full file search done on this structure

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE
L4 SCR 2039 - abnormal mass - all isotopic specifications
L6 SCR 2045 OR 2046 - hydrogen isotopes (excluded from answer set)
L8 35 SEA FILE=REGISTRY SSS FUL L3 AND L4 NOT L6
L11 STR

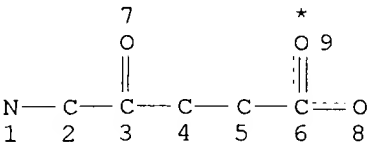


the following 3 structures L11, L12, L13 were removed from the answer set (all contain isotopic oxygen)

NODE ATTRIBUTES:
MASS IS * AT 7
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 9

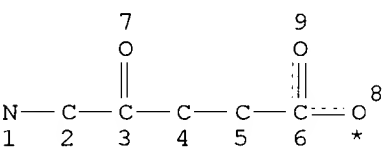
STEREO ATTRIBUTES: NONE
L12 STR



NODE ATTRIBUTES:
MASS IS * AT 9
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE
L13 STR



NODE ATTRIBUTES:
MASS IS * AT 8
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE
L15 29 SEA FILE=REGISTRY SUB=L8 SSS FUL (L3 NOT ((L11 OR L12 OR L13)))

100.0% PROCESSED 35 ITERATIONS 29 ANSWERS
SEARCH TIME: 00.00.01

FILE 'CAPLUS' ENTERED AT 16:44:14 ON 16 JAN 2001
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1967 - 16 Jan 2001 VOL 134 ISS 4
FILE LAST UPDATED: 15 Jan 2001 (20010115/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

Searched by Barb O'Bryen, STIC 308-4291

This file supports REGistRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

Now you can extend your author, patent assignee, patent information, and title searches back to 1907. The records from 1907-1966 now have this searchable data in CAOLD. You now have electronic access to all of CA: 1907 to 1966 in CAOLD and 1967 to the present in CAPLUS on STN.

The CA Lexicon is now available in the Controlled Term (/CT) field. Enter HELP LEXICON for full details.

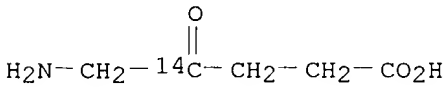

```
L3              STR
L4              SCR 2039
L6              SCR 2045 OR 2046
L8           35 SEA FILE=REGISTRY SSS FUL L3 AND L4 NOT L6
L11             STR
L12             STR
L13             STR
L15          29 SEA FILE=REGISTRY SUB=L8 SSS FUL (L3 NOT ((L11 OR L12 OR
                L13)))
L16          45 SEA FILE=CAPLUS ABB=ON  L15
```

```
=> d ibib abs hitstr l16 1-45; fil cao; d que nos l17
```

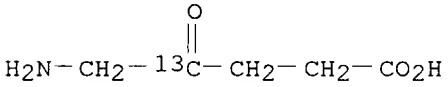
display format prints Registry records after matching citations

```
L16  ANSWER 1 OF 45  CAPLUS  COPYRIGHT 2001 ACS
ACCESSION NUMBER:         1999:235942  CAPLUS
DOCUMENT NUMBER:          131:167488
TITLE:                    Biosynthesis of porphyrins and related macrocycles.
                          Part 51. Proof that a reductive step occurs during the
                          biosynthesis of vitamin B12 by the microaerophilic
                          organism, Propionibacterium shermanii
AUTHOR(S):                Ichinose, Koji; Kodera, Masahito; Leeper, Finian J.;
                          Battersby, Alan R.
CORPORATE SOURCE:         University Chemical Laboratory, Cambridge, CB2 1EW, UK
SOURCE:                   J. Chem. Soc., Perkin Trans. 1 (1999), (8), 879-888
                          CODEN: JCPRB4; ISSN: 0300-922X
PUBLISHER:                Royal Society of Chemistry
DOCUMENT TYPE:            Journal
LANGUAGE:                 English
AB   5-Amino[4-13C]levulinic acid was synthesized for enzymic conversion into
     13C-labeled precorrin-2. This was incubated with an enzyme system from P.
     shermanii in the presence of [4-2H2]NADH and [4-2H2]NADPH to yield
     cobyrinic acid, shown to carry 2H at C-19 by appropriate 13C-NMR studies.
     The same reducing cofactors but now stereospecifically labeled at C-4 with
     3H were similarly used to biosynthesize cobyrinic acid which was
     3H-labeled from the 4(R)-cofactors but carried no 3H when the
     4(S)-cofactors were used. Suitable degrdn. of the cobyrinic acid after
     conversion into its ester proved 3H-labeling at C-19. These results
     establish that the biosynthesis of vitamin B12 in the microaerophilic
     organism P. shermanii involves a reductive step in which a reductase
     enzyme transfers 4-HR of the cofactor to C-19 of the macrocycle.
IT   16387-80-7P 129720-94-1P
                          Searched by Barb O'Bryen, STIC  308-4291
```

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 16387-80-7 CAPLUS
CN Pentanoic-4-14C acid, 5-amino-4-oxo-, hydrochloride (9CI) (CA INDEX NAME)



RN 129720-94-1 CAPLUS
CN Pentanoic-4-13C acid, 5-amino-4-oxo-, hydrochloride (9CI) (CA INDEX NAME)



REFERENCE COUNT: 29
REFERENCE(S):
(1) Abell, C; J Chem Soc Chem Commun 1981, P856 CAPLUS
(2) Balachandran, S; J Chem Soc Perkin Trans 1 1994, P487 CAPLUS
(3) Bartels, G; Liebigs Ann Chem 1979, P1440 CAPLUS
(6) Battersby, A; J Chem Soc Chem Commun 1984, P527 CAPLUS
(7) Battersby, A; J Chem Soc, Perkin Trans 1 1977, P158 CAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 2 OF 45 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1999:9731 CAPLUS
DOCUMENT NUMBER: 130:78111
TITLE: Diagnostic agents and remedies for malignant tumors
INVENTOR(S): Tanaka, Tohru; Sasaki, Hiroshi
PATENT ASSIGNEE(S): Cosmo Research Institute, Japan; Cosmo Oil Co., Ltd.
SOURCE: PCT Int. Appl., 23 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

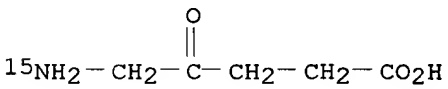
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9857668	A1	19981223	WO 1998-JP2648	19980616
W: CA, NO, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
JP 11012197	A2	19990119	JP 1997-160945	19970618
EP 995448	A1	20000426	EP 1998-924643	19980616
R: DE, FR, GB				
NO 9906253	A	20000218	NO 1999-6253	19991216

PRIORITY APPLN. INFO.: JP 1997-160945 19970618
WO 1998-JP2648 19980616

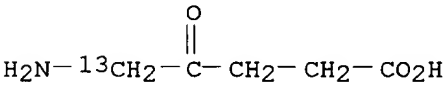
AB Diagnostic agents or photodynamic remedies for malignant tumors contg. as the active ingredient compds. wherein at least one carbon atom of 5-aminolevulinic acid is a carbon isotope or the nitrogen atom in the amino group thereof is a nitrogen isotope, esters, amides or salts of these compds. or hydrates or solvates thereof.

IT **60556-69-6P 79503-87-0P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(radioisotope-labeled 5-aminolevulinic salts as diagnostic agents and remedies for malignant tumors)

RN 60556-69-6 CAPLUS
CN Pentanoic acid, 5-(amino-15N)-4-oxo- (9CI) (CA INDEX NAME)



RN 79503-87-0 CAPLUS
CN Pentanoic-5-13C acid, 5-amino-4-oxo- (9CI) (CA INDEX NAME)



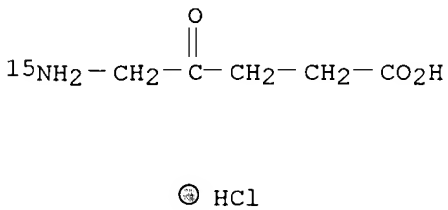
REFERENCE COUNT: 7
REFERENCE(S):
(1) Anon; EP 845457 A1 CAPLUS
(2) Cosmo Research Institute, Cosmo Oil Co, Ltd; JP 04-9360 A 1992 CAPLUS
(3) Hua, Z; Cancer Res V55(8), P1723 CAPLUS
(4) Mitsubishi Chemical Corp; WO 97/03042 A1 1997 CAPLUS
(5) Nippon Oil Co, Ltd; JP 05-38294 A 1993 CAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 3 OF 45 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1997:659247 CAPLUS
DOCUMENT NUMBER: 127:293588
TITLE: Synthesis of .delta.-[15N]aminolevulinic acid hydrochloride
AUTHOR(S): Iida, Katsumi; Takao, Yuki; Ogai, Tomoe; Kajiwara, Masahiro
CORPORATE SOURCE: Department of Medicinal Chemistry, Meiji College of Pharmacy, Tanashi, 188, Japan
SOURCE: J. Labelled Compd. Radiopharm. (1997), 39(10), 797-802
CODEN: JLCRD4; ISSN: 0362-4803
PUBLISHER: Wiley
DOCUMENT TYPE: Journal
LANGUAGE: English

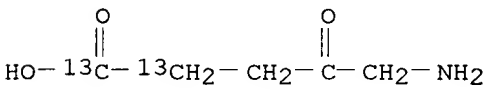
AB .delta.-[15N]aminolevulinic acid hydrochloride was synthesized in high yield by condensation of potassium [15N]phthalimide and tetrahydrofurfuryl bromide, followed by ruthenium oxidn. and hydrolysis. Relevant 15N-NMR spectral data are presented.

IT **116571-80-3**
RL: RCT (Reactant)
(synthesis of nitrogen-labeled aminolevulinic acid hydrochloride)

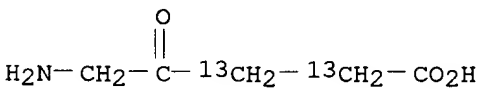
RN 116571-80-3 CAPLUS
CN Pentanoic acid, 5-(amino-15N)-4-oxo-, hydrochloride (9CI) (CA INDEX NAME)



L16 ANSWER 4 OF 45 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1997:507923 CAPLUS
DOCUMENT NUMBER: 127:191034
TITLE: Synthesis of [1,2-13C]- and [2,3-13C]-labeled .delta.-aminolevulinic acid
AUTHOR(S): Bunce, Richard A.; Schilling, Curtis L., III; Rivera, Mario
CORPORATE SOURCE: Department of Chemistry, Oklahoma State University, Stillwater, OK, 74078-3071, USA
SOURCE: J. Labelled Compd. Radiopharm. (1997), 39(8), 669-675
CODEN: JLCRD4; ISSN: 0362-4803
PUBLISHER: Wiley
DOCUMENT TYPE: Journal
LANGUAGE: English
AB [1,2-13C]- and [2,3-13C]-labeled .delta.-aminolevulinic acids (H2NCH2COCH2CH2CO2H; .delta.-ALA) have been prepd. by a four-step sequence. [1,2-13C]-Et bromoacetate was used to introduce the labels in the 1,2-labeled .delta.-ALA while [2-13C]-Et bromoacetate and [5-13C]-Meldrum's acid were used to introduce the labels in the 2,3-labeled deriv. These amino acid building blocks can be used to prep. heme-contg. proteins with labeled hemes according to previously reported biosynthetic method.
IT **194469-35-7P 194469-36-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of doubly 13C-labeled .delta.-aminolevulinic acids)
RN 194469-35-7 CAPLUS
CN Pentanoic-1,2-13C2 acid, 5-amino-4-oxo-, hydrochloride (9CI) (CA INDEX NAME)

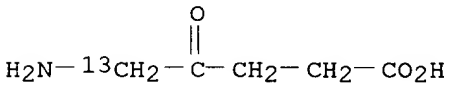


RN 194469-36-8 CAPLUS
CN Pentanoic-2,3-13C2 acid, 5-amino-4-oxo-, hydrochloride (9CI) (CA INDEX NAME)



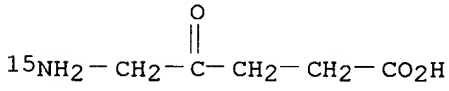
● HCl

L16 ANSWER 5 OF 45 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1997:269694 CAPLUS
DOCUMENT NUMBER: 126:293223
TITLE: An efficient synthesis of .delta.-aminolevulinic acid (ALA) and its isotopomers. [Erratum to document cited in CA126:171421]
AUTHOR(S): Wang, Jianji; Scott, A. Ian
CORPORATE SOURCE: Dep. Chemistry, Texas A&M Univ., College Station, TX, 77843-3255, USA
SOURCE: Tetrahedron Lett. (1997), 38(15), 2587
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The authors regret that an important ref. to an earlier and similar approach to 5-aminolevulinic acid was inadvertently omitted from this paper.
IT **52065-79-9P 116571-80-3P 129720-94-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(efficient prepn. of .delta.-aminolevulinic acid and its isotopomers from labeled glycine (Erratum))
RN 52065-79-9 CAPLUS
CN Pentanoic-5-13C acid, 5-amino-4-oxo-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

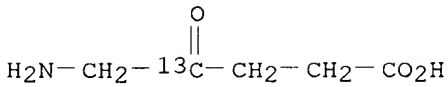
RN 116571-80-3 CAPLUS
CN Pentanoic acid, 5-(amino-15N)-4-oxo-, hydrochloride (9CI) (CA INDEX NAME)



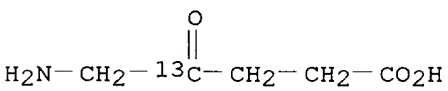
● HCl

RN 129720-94-1 CAPLUS
CN Pentanoic-4-13C acid, 5-amino-4-oxo-, hydrochloride (9CI) (CA INDEX NAME)

Searched by Barb O'Bryen, STIC 308-4291

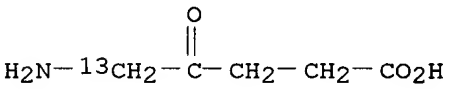


L16 ANSWER 6 OF 45 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1997:108749 CAPLUS
DOCUMENT NUMBER: 126:225514
TITLE: Enzymic synthesis of S-adenosyl-L-methionine on the preparative scale
AUTHOR(S): Park, Jeongho; Tai, Junzhe; Roessner, Charles A.; Scott, A. Ian
CORPORATE SOURCE: Center for Biological NMR, Department of Chemistry, Texas AandM University, College Station, TX, 77843-3255, USA
SOURCE: Bioorg. Med. Chem. (1996), 4(12), 2179-2185
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The problems inherent in the enzymic and chem. synthesis of S-adenosyl-L-methionine (SAM) led to development of an efficient, simple method for the synthesis of large amts. of labeled SAM. It has previously been reported that the problem of product inhibition of E. coli SAM synthetase encoded by the metK gene was successfully overcome in the presence of sodium p-toluenesulfonate (pTsONa). This research has now been expanded to demonstrate that product inhibition of this enzyme can also be overcome by adding a high concn. of .beta.-mercaptoethanol (.beta.ME), acetonitrile, or urea. In addn., a recombinant strain of E. coli has been constructed that expresses the yeast SAM synthetase encoded by the sam2 gene. The yeast enzyme does not have the problem of product inhibition seen with the E. coli enzyme. Complete conversion of 10 mM methionine to SAM was achieved in incubations with either the recombinant yeast enzyme and 1 M potassium ion or the E. coli enzyme in the presence of additives such as .beta.ME, acetonitrile, urea, or pTsONa. The recombinant yeast SAM synthetase was used to generate SAM in situ for use in the multi-enzymic synthesis of precorrin 2.
IT **114791-06-9**
RL: RCT (Reactant)
(enzymic synthesis of S-adenosyl-L-methionine on the preparative scale)
RN 114791-06-9 CAPLUS
CN Pentanoic-4-13C acid, 5-amino-4-oxo- (9CI) (CA INDEX NAME)



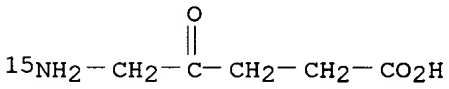
L16 ANSWER 7 OF 45 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1997:105596 CAPLUS
DOCUMENT NUMBER: 126:171421
TITLE: An efficient synthesis of .delta.-aminolevulinic acid (ALA) and its isotopomers
AUTHOR(S): Wang, Jianji; Scott, A. Ian
CORPORATE SOURCE: Dep. Chemistry, Texas A&M Univ., College Station, TX, Searched by Barb O'Bryen, STIC 308-4291

77843-3255, USA
SOURCE: Tetrahedron Lett. (1997), 38(5), 739-740
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A new and improved synthesis of 13C-4-, 13C-5- and 15N-.delta.-aminolevulinic acid (ALA), with 90% overall yield in 4 steps from labeled glycine, is described.
IT **52065-79-9P 116571-80-3P 129720-94-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(efficient prepn. of .delta.-aminolevulinic acid and its isotopomers from labeled glycine)
RN 52065-79-9 CAPLUS
CN Pentanoic-5-13C acid, 5-amino-4-oxo-, hydrochloride (9CI) (CA INDEX NAME)



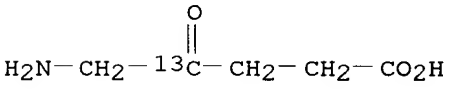
● HCl

RN 116571-80-3 CAPLUS
CN Pentanoic acid, 5-(amino-15N)-4-oxo-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

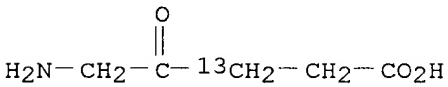
RN 129720-94-1 CAPLUS
CN Pentanoic-4-13C acid, 5-amino-4-oxo-, hydrochloride (9CI) (CA INDEX NAME)



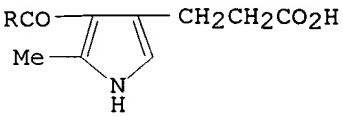
● HCl

L16 ANSWER 8 OF 45 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1995:827143 CAPLUS
DOCUMENT NUMBER: 123:222020
TITLE: Biosynthetic preparation of isotopically labeled heme
AUTHOR(S): Rivera, Mario; Walker, F. Ann
CORPORATE SOURCE: Dep. Chem., Oklahoma State Univ., Stillwater, OK, 74074, USA
SOURCE: Anal. Biochem. (1995), 230(2), 295-302
CODEN: ANBCA2; ISSN: 0003-2697
Searched by Barb O'Bryen, STIC 308-4291

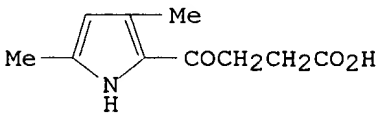
DOCUMENT TYPE: Journal
LANGUAGE: English
AB An efficient method for the prepn. of isotopically enriched heme was developed. This method utilizes a com. available bacterial host and plasmid, into which a synthetic gene encoding for rat liver outer mitochondrial membrane cytochrome b5, a heme-binding protein, was inserted. The method uses the efficient synthesis of the cytochrome b5 polypeptide together with the enhanced biosynthesis of heme brought about by addn. of the first committed precursor in heme biosynthesis, .delta.-aminolevulinic acid. Apocytochrome b5 sequesters heme as the macrocycle is being synthesized to form holocytochrome b5, thus avoiding toxic concns. of free macrocycle in the cell. Relatively high concns. of free heme in the cell have been shown to stimulate excretion of heme precursors such as coproporphyrinogen and uroporphyrinogen (W. F. Harris III et al., 1993), therefore causing isotopic diln. of the labeled material. The heme obtained by this methodol. was >85% enriched. Because the heme in cytochrome b5 is not covalently attached to the polypeptide, it can be extd. and used in other applications. Use of glutamate, a precursor of .delta.-aminolevulinate biosynthesis in Escherichia coli, did not result in high levels of isotopic incorporation into heme, thus pointing out the importance of using a labeled precursor that is committed to heme biosynthesis to obtain high levels of isotopic labeling.
IT **123253-93-0**
RL: BPR (Biological process); BIOL (Biological study); PROC (Process)
(biosynthetic prepn. of isotopically labeled heme)
RN 123253-93-0 CAPLUS
CN Pentanoic-3-13C acid, 5-amino-4-oxo- (9CI) (CA INDEX NAME)



L16 ANSWER 9 OF 45 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1994:190778 CAPLUS
DOCUMENT NUMBER: 120:190778
TITLE: Mechanism of acid catalysis in the cyclization of 5-aminolevulinic acid and acetylacetone to 3-acetyl-4-(2-carboxyethyl)-2-methylpyrrole
AUTHOR(S): Butler, Anthony R.; George, Sharon D.
CORPORATE SOURCE: Sch. Chem., Univ. St. Andrews, St. Andrews, KY16 9ST, UK
SOURCE: J. Chem. Soc., Perkin Trans. 2 (1994), (2), 315-18
CODEN: JCPKBH; ISSN: 0300-9580
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



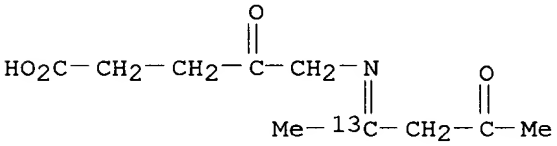
II

AB Under acid conditions 5-aminolevulinic acid reacts with acetylacetone to give the title heterocycle (I, R = Me). There is also formation of a small amt. of the Fischer-Fink product (II). 13C and 15N NMR spectroscopy showed that the first condensation product to accumulate is an enamino ketone (III). The trifluoro analog of III was isolated, and its cyclization to I (R = CF3) was monitored. There is a substantial spontaneous reaction, and the acid-catalyzed process occurs by specific acid catalysis.

IT **153695-89-7P**
RL: PRP (Properties); FORM (Formation, nonpreparative); PREP (Preparation) (formation and NMR of)

RN 153695-89-7 CAPLUS

CN Pentanoic acid, 5-[(1-methyl-3-oxobutylidene-1-13C)amino]-4-oxo- (9CI) (CA INDEX NAME)



L16 ANSWER 10 OF 45 CAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1994:185710 CAPLUS

DOCUMENT NUMBER: 120:185710

TITLE: Biosynthesis of porphyrins and related macrocycles. Part 41. Fate of oxygen atoms as precorrin-2 carrying eight labeled carboxyl groups (13C18O2H) is enzymically converted to cobyrinic acid

AUTHOR(S): Vishwakarma, Ram A.; Balachandran, Sarala; Alanine, Alex I. D.; Stamford, N. Patrick J.; Kiuchi, Fumiyuki; Leeper, Finian J.; Battersby, Alan R.

CORPORATE SOURCE: Univ. Chem. Lab., Cambridge, CB2 1EW, UK

SOURCE: J. Chem. Soc., Perkin Trans. 1 (1993), (23), 2893-9
CODEN: JCPRB4; ISSN: 0300-922X

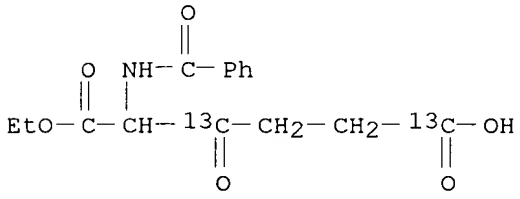
DOCUMENT TYPE: Journal

LANGUAGE: English

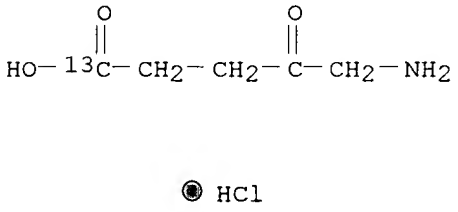
AB 5-Amino[1,4-13C2]levulinic acid and 5-amino[1-13C]levulinic acid are synthesized and all three 16O atoms of the latter are exchanged for 18O. The 13C,18O-labeled material is then converted in vitro into precorrin-2 by the combined action of four genetically overproduced enzymes. The product is isolated in its aromatized form, sirohydrochlorin (I) and 13C-NMR shows that all 8 carboxyl groups of I retain both oxygen atoms throughout the biosynthesis. A cell-free enzyme prepn. from Propionibacterium shermanii converts the 13C,18O-labeled I via precorrin-2 into cobyrinic acid, a late precursor of vitamin B12. 13C-NMR proves that 6 carboxyl groups of cobyrinic acid retain both oxygen atoms whereas the

a-carboxyl group undergoes specific loss of one labeled oxygen atom.

IT **153598-25-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and conversion to aminolevulinate)
RN 153598-25-5 CAPLUS
CN Hexanedioic-1,4-13C2 acid, 5-(benzoylamino)-4-oxo-, 6-ethyl ester (9CI) (CA INDEX NAME)

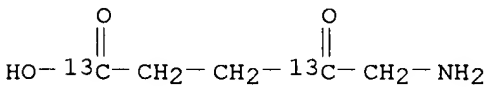


IT **106213-17-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and oxygen-18 exchange reaction of)
RN 106213-17-6 CAPLUS
CN Pentanoic-1-13C acid, 5-amino-4-oxo-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

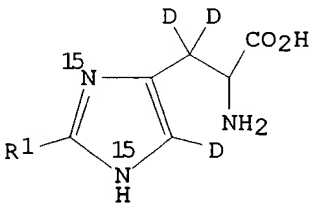
IT **153598-23-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 153598-23-3 CAPLUS
CN Pentanoic-1,4-13C2 acid, 5-amino-4-oxo-, hydrochloride (9CI) (CA INDEX NAME)



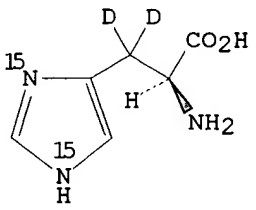
○ HCl

L16 ANSWER 11 OF 45 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1992:612904 CAPLUS
DOCUMENT NUMBER: 117:212904
TITLE: Synthesis of selectively multi-labeled histidines with stable isotopes and chiral synthesis of L-histidine from L-aspartic acid
AUTHOR(S): Furuta, Takashi; Katayama, Motofusa; Shibasaki, Hiromi; Kasuya, Yasuji
CORPORATE SOURCE: Clin. Pharm., Tokyo Coll. Pharm., Hachioji, 192-03, Japan
Searched by Barb O'Bryen, STIC 308-4291

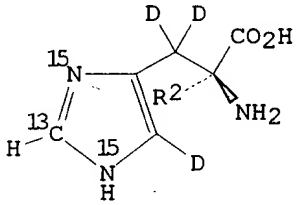
SOURCE: J. Chem. Soc., Perkin Trans. 1 (1992), (13), 1643-8
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



II



III



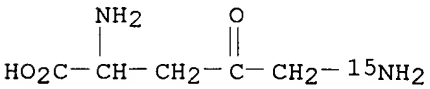
IV

AB An efficient and concise synthesis of three types of multiple-labeled histidines with stable isotopes to be used for investigating pharmacokinetics and enzymic reaction mechanisms in vivo is described. Selective deuteration at C-3 and C-5 of diamino acid DL-H215NCR2COCR2CH(NH2)CO2H (I; R = H) was achieved by hydrogen exchange to give tetradeuterated acid I (R = D). The imidazole ring was constructed by heating of I (R = D) with NaSC15N in D2O to give labeled 2'-mercapto-DL-histidine DL-II (R1 = SH), which was oxidized at C-2' to give the desired histidine L-II (R1 = H) after enzymic resoln. To replace deuterium at C-5' with hydrogen, the labeled histidine DL-II (R1 = H) was heated in water (pH 5.0) at 180.degree., and subsequent enzymic resoln. gave III. A similar sequence of reactions carried out on the diamino acid I (R = D) with KS13C15N gave DL-IV (R2 = H). Deuteration at C-2 and C-2' of DL-IV (R2 = H) with DCl-D2O (pD 5.0) at 180.degree. and subsequent back-exchange of deuterium at C-2' with water (pH 7.0) at 120.degree. gave DL-IV (R2 = D). Synthesis of optically pure L-histidine starting from L-aspartic acid is also described. The optical purity of the synthesized L-histidine was estd. to be 93.8% enantiomeric excess.

IT **143687-01-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and deuteration of, tetradeuterio analog from)

RN 143687-01-8 CAPLUS

CN Ornithine-N5-15N, 4-oxo-, dihydrochloride (9CI) (CA INDEX NAME)



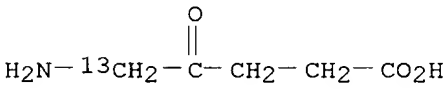
●2 HCl

L16 ANSWER 12 OF 45 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1992:37407 CAPLUS
DOCUMENT NUMBER: 116:37407
TITLE: Enzymic synthesis and structure of precorrin-3, a trimethyldipyrrocorphin intermediate in vitamin B12 biosynthesis
AUTHOR(S): Warren, Martin J.; Roessner, Charles A.; Ozaki, Shinichi; Stolowich, Neal J.; Santander, Patricio J.; Scott, A. Ian
CORPORATE SOURCE: Cent. Biol. NMR, Texas A and M Univ., College Station, TX, 77843-3255, USA
SOURCE: Biochemistry (1992), 31(2), 603-9
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English

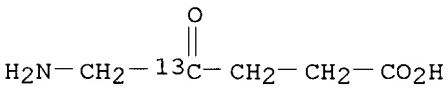
AB The trimethylated intermediate of vitamin B12 (corrin) biosynthesis, precorrin-3, was produced from various 13C-enriched isotopomers of 5-aminolevulinic acid by using a multiple-enzyme system contg. aminolevulinic acid dehydratase, porphobilinogen deaminase uroporphyrinogen (uro'gen) III synthetase, and the S-adenosyl-L-methionine (SAM-) dependent uro'gen III methyltransferase and precorrin-2 methyltransferase in the presence of [13C]SAM. Structural anal. of the resulting product, precorrin-3, reveals a close similarity to precorrin-2 but with several subtle differences in the conjugated array of C:C and C:N bonds that reflect the presence of the new C-Me group at C20 and its influence on the electronic distribution in the dipyrrocorphin chromophore. The implications of this structure for corrin biosynthesis are discussed.

IT **79503-87-0 114791-06-9 123253-93-0**
RL: ANST (Analytical study)
(in precorrin enzymic prepn.)

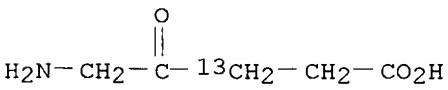
RN 79503-87-0 CAPLUS
CN Pentanoic-5-13C acid, 5-amino-4-oxo- (9CI) (CA INDEX NAME)



RN 114791-06-9 CAPLUS
CN Pentanoic-4-13C acid, 5-amino-4-oxo- (9CI) (CA INDEX NAME)



RN 123253-93-0 CAPLUS
CN Pentanoic-3-13C acid, 5-amino-4-oxo- (9CI) (CA INDEX NAME)



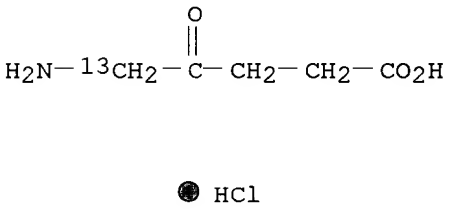
L16 ANSWER 13 OF 45 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1991:19952 CAPLUS
Searched by Barb O'Bryen, STIC 308-4291

DOCUMENT NUMBER: 114:19952
TITLE: Biosynthesis of porphyrins and related macrocycles. Part 35. Discovery of a novel dipyrrolic cofactor essential for the catalytic action of hydroxymethylbilane synthase (porphobilinogen deaminase)
AUTHOR(S): Hart, Graham J.; Miller, Andrew D.; Beifuss, Uwe; Leeper, Finian J.; Battersby, Alan R.
CORPORATE SOURCE: Univ. Chem. Lab., Cambridge, CB2 1EW, UK
SOURCE: J. Chem. Soc., Perkin Trans. 1 (1990), (7), 1979-93
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Hydroxymethylbilane synthase constructs the open-chain hydroxymethylbilane by assembly of 4 porphobilinogen units head-to-tail, the first of these being covalently bound to the enzyme through a group X. The surprising discovery is made that X is a novel dipyrromethane cofactor constructed from 2 porphobilinogen units and bound to the protein via the S of cysteine. This cofactor does not turn over in the catalytic process but acts as an anchor for the assembly of hexapyrrole from which the tetrapyrrolic hydroxymethylbilane is cleaved leaving the dipyrromethane cofactor in place for a further building cycle.

IT **52065-79-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and porphobilinogen deaminase dipyromethane cofactor formation from)

RN 52065-79-9 CAPLUS
CN Pentanoic-5-13C acid, 5-amino-4-oxo-, hydrochloride (9CI) (CA INDEX NAME)



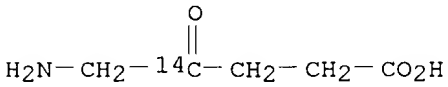
L16 ANSWER 14 OF 45 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1990:628049 CAPLUS
DOCUMENT NUMBER: 113:228049
TITLE: Radiolabeling of chlorophyll for studies on catabolism
AUTHOR(S): Peisker, Christian; Thomas, Howard; Keller, Felix; Matile, Philippe
CORPORATE SOURCE: Dep. Plant Biol., Univ. Zurich, Zurich, CH-8008, Switz.
SOURCE: J. Plant Physiol. (1990), 136(5), 544-9
CODEN: JPPHEY; ISSN: 0176-1617
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A technique for specifically radiolabelling chlorophyll (Chl) during greening of etiolated barley seedlings is described. Both detached shoots and intact seedlings were employed. Shoots were pretreated with gabaculine, an inhibitor of the reversible .delta.-aminolevulinic acid (ALA)-synthesizing transaminase, and then exposed to low light levels in the presence of 4[14C]-ALA. Radioactivity in ALA labeled in the 4-position is locked into the pyrrole rings of porphyrin. Under these circumstances, 80-90% of the total label incorporated during greening was sol. in 80% acetone and of the acetone-sol. radioactivity over 70% was extractable with hexane and recovered in Chl a and b. The feeding of ALA

via the rootlets of whole seedlings yielded the same pattern of labeling. It did not require the presence of gabaculine and was assocd. with a better reproducibility of uptake and total incorporation of radioactivity than expts. with detached shoots. Upon the induction of senescence, radioactivity gradually disappeared from the Chls and appeared in a no. of polar compds. Two of them turned out to be identical with putative nongreen catabolites described earlier.

IT **7729-71-7**
RL: BIOL (Biological study)
(radiolabeling of chlorophyll with, during greening of etiolated barley seedlings, for studies on catabolism)

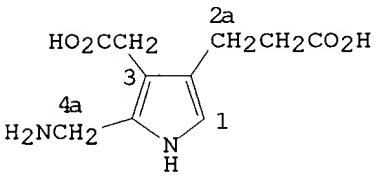
RN 7729-71-7 CAPLUS
CN Pentanoic-4-14C acid, 5-amino-4-oxo- (9CI) (CA INDEX NAME)



L16 ANSWER 15 OF 45 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1990:553043 CAPLUS
DOCUMENT NUMBER: 113:153043
TITLE: Preparation of 13C-labeled 5-aminolevulinic acid
INVENTOR(S): Kajiwara, Masahiro
PATENT ASSIGNEE(S): Nippon Steel Chemical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 02111747	A2	19900424	JP 1988-263877	19881021

GI



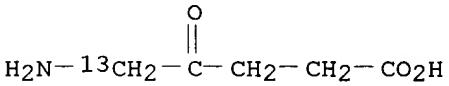
V

AB 1-, 3-, 4- Or 5-13C-labeled 5-aminolevulinic acid (I), useful in diagnosis or study of biosynthesis and metab. by 13C-NMR, is prepd. from [1- and/or 2-13C] AcONa (II) via intermediates BrCH2CO2Et (III), (2,2-dimethyl-1,3-dioxane-4,6-dione), and N-phthaloylglycine (IV) and is further condensed in the presence of a dehydratase to give 13C-labeled porphobilinogen (V). Thus, a soln. of IV Et ester in MeOCH2CH2OMe (DME) was added to a suspension of NaH in DME and after stirring 1 h a DME soln. of [1-13C]III added, the mixt. was stirred 1 day to give [1-13C]Et 3-ethoxycarbonyl-N-phthaloyllevulinate which was hydrolyzed with AcOH/concd. HCl (1:1) under reflux to give [1-13C]I. HCl. [3-13C]- and [5-13C] I prepd. from [2-13C]BrCH2CO2H and [2-13C]glycine, resp., were stirred with

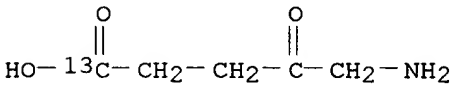
aminolevulinate dehydratase in a phosphate buffer contg. ZnSO4-dithiothreitol to give [2a,3-13C] and [2,4a-13C] I, resp.

IT **52065-79-9P 106213-17-6P 129720-94-1P 129720-95-2P 129720-96-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as intermediate for 13C-labeled porphobilinogen)

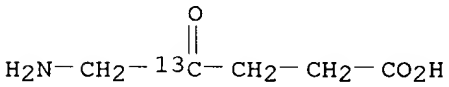
RN 52065-79-9 CAPLUS
CN Pentanoic-5-13C acid, 5-amino-4-oxo-, hydrochloride (9CI) (CA INDEX NAME)



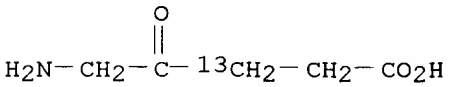
RN 106213-17-6 CAPLUS
CN Pentanoic-1-13C acid, 5-amino-4-oxo-, hydrochloride (9CI) (CA INDEX NAME)



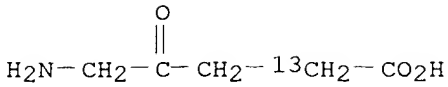
RN 129720-94-1 CAPLUS
CN Pentanoic-4-13C acid, 5-amino-4-oxo-, hydrochloride (9CI) (CA INDEX NAME)



RN 129720-95-2 CAPLUS
CN Pentanoic-3-13C acid, 5-amino-4-oxo-, hydrochloride (9CI) (CA INDEX NAME)



RN 129720-96-3 CAPLUS
CN Pentanoic-2-13C acid, 5-amino-4-oxo-, hydrochloride (9CI) (CA INDEX NAME)

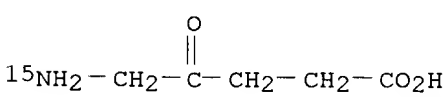


L16 ANSWER 16 OF 45 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1990:528599 CAPLUS
DOCUMENT NUMBER: 113:128599
TITLE: Nitrogen-15 and carbon-13 NMR studies of ligands bound to the 280 000-dalton protein porphobilinogen synthase elucidate the structures of enzyme-bound product and a Schiff base intermediate
AUTHOR(S): Jaffe, Eileen K.; Markham, George D.; Rajagopalan, Jayanthi S.
CORPORATE SOURCE: Sch. Dent. Med., Univ. Pennsylvania, Philadelphia, PA, 19104-6002, USA
SOURCE: Biochemistry (1990), 29(36), 8345-50
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Porphobilinogen synthase (PBGS) catalyzes the asym. condensation of 2 mols. of 5-aminolevulinic acid (ALA). Despite the 280,000-dalton size of PBGS, much can be learned about the reaction mechanism through 13C and 15N NMR. These studies may represent the largest protein complex for which individual nuclei have been characterized by 13C or 15N NMR. Here, 13C NMR studies are extended to PBGS complexes with [3,3-2H2,3-13C]ALA and 15N NMR studies of [15N]ALA bound to PBGS are reported. As in previous 13C NMR studies, observation of enzyme-bound 15N-labeled species was facilitated by deuteration at N atoms that are attached to slowly exchanging H atoms. For holo-PBGS at neutral pH, the NMR spectra reflected the structure of the enzyme-bound product porphobilinogen (PBG), whose chem. shifts were uniformly consistent with deprotonation of the NH2 group whose soln. pKa is 11. Despite this local environment, the protons of the NH2 group were in rapid exchange with solvent (kexchange > 102 s-1). For Me methanethiosulfonate (MMTS)-modified PBGS, the NMR spectra reflected the chem. of an enzyme-bound Schiff base intermediate that was formed between C4 of ALA and an active-site lysine. The 13C chem. shift of [3,3-2H2,3-13C]ALA confirmed that the Schiff base is an imine of E stereochem. By comparison to model imines formed between [15N]ALA and hydrazine or hydroxylamine, the 15N chem. shift of the enzyme-bound Schiff base suggested that the free NH2 group is in an environment resembling partial deprotonation; again the protons were in rapid exchange with solvent. Deprotonation of the NH2 group would facilitate formation of a Schiff base between the NH2 group of the enzyme-bound Schiff base and C4 of the 2nd ALA substrate. This is the 1st evidence supporting C-N bond formation as the initial site of interaction between the 2 substrate mols.

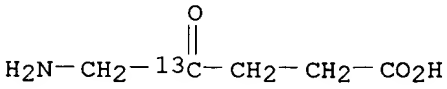
IT **60556-69-6 114791-06-9 123253-93-0**
RL: RCT (Reactant)
(reaction of, with porphobilinogen synthase of liver, NMR study of)

RN 60556-69-6 CAPLUS
CN Pentanoic acid, 5-(amino-15N)-4-oxo- (9CI) (CA INDEX NAME)

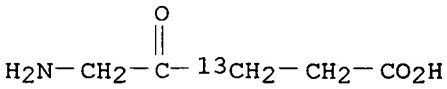


Searched by Barb O'Bryen, STIC 308-4291

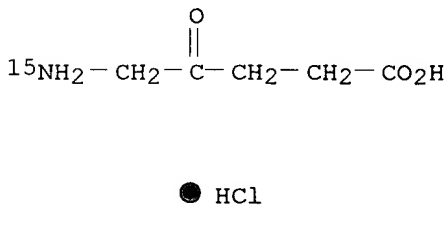
RN 114791-06-9 CAPLUS
CN Pentanoic-4-13C acid, 5-amino-4-oxo- (9CI) (CA INDEX NAME)



RN 123253-93-0 CAPLUS
CN Pentanoic-3-13C acid, 5-amino-4-oxo- (9CI) (CA INDEX NAME)



L16 ANSWER 17 OF 45 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1990:494527 CAPLUS
DOCUMENT NUMBER: 113:94527
TITLE: Studies on the biosynthesis of corrinoids and porphyrinoids. II. The origin of nitrogen of vitamin B12
AUTHOR(S): Kurumaya, Katsuyuki; Okazaki, Takeo; Kajiwara, Masahiro
CORPORATE SOURCE: Dep. Med. Chem., Meiji Coll. Pharm., Tanashi, 188, Japan
SOURCE: Chem. Pharm. Bull. (1990), 38(4), 1058-61
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
AB To clarify the origin of N of vitamin B12, 15N-labeled aminolevulinic acid (ALA) was prepd. and administered to Propionibacterium shermanii. Vitamin B12 thus isolated showed 4 signals in the 15N-NMR spectrum. The N of [5-15N]riboflavin was incorporated into the benzimidazole part of vitamin B12. Hydroxycobalamin was transformed into cyanocobalamin by treatment with KC15N, and the 15N-NMR spectrum was measured. The results of these expts. revealed the origin of the N of vitamin B12 and allowed the 15N-NMR signals to be assigned.
IT **116571-80-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 116571-80-3 CAPLUS
CN Pentanoic acid, 5-(amino-15N)-4-oxo-, hydrochloride (9CI) (CA INDEX NAME)



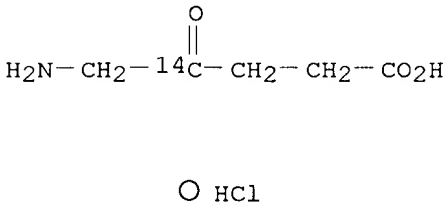
L16 ANSWER 18 OF 45 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1990:406765 CAPLUS
DOCUMENT NUMBER: 113:6765
Searched by Barb O'Bryen, STIC 308-4291

TITLE: A short synthesis of 5-amino[4-14C]levulinic acid hydrochloride
AUTHOR(S): Campbell, J. B.; Johnston, J. S.
CORPORATE SOURCE: Amersham Int. PLC, Cardiff, CF4 7YT, UK
SOURCE: J. Labelled Compd. Radiopharm. (1989), 27(12), 1353-8
CODEN: JLCRD4; ISSN: 0362-4803
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 113:6765

AB The title compd. was prepd. from K14CN in 56% overall yield. The key step is the Pd(0)-catalyzed coupling of 2-phthalimido[1-14C]acetyl chloride with EtO2CCH2CH2ZnI to give 5-phthalimido[4-14C]levulinic acid Et ester in 86% yield. The synthesis was carried out at high specific activity from 720 mCi of starting material.

IT **16387-80-7P**, 5-Amino[4-14C]levulinic acid hydrochloride
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 16387-80-7 CAPLUS
CN Pentanoic-4-14C acid, 5-amino-4-oxo-, hydrochloride (9CI) (CA INDEX NAME)



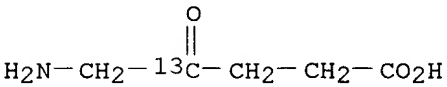
L16 ANSWER 19 OF 45 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1990:134583 CAPLUS
DOCUMENT NUMBER: 112:134583
TITLE: Biosynthesis of chlorophyll and bacteriochlorophyll
AUTHOR(S): Okazaki, Takeo; Sagae, Yoko; Kurumaya, Katsuyuki; Kajiwara, Masahiro
CORPORATE SOURCE: Dep. Med. Chem., Meiji Coll. Pharm., Japan
SOURCE: Tennen Yuki Kagobutsu Toronkai Koen Yoshishu (1989), 31st, 677-84
CODEN: TYKYDS
DOCUMENT TYPE: Journal
LANGUAGE: Japanese

AB 13C-labeled precursors such as glycine, methionine, and glutamic acid were synthesized for the biosynthesis of porphyrinoid. The regioselective synthesis of 13-labeled ALA (.delta.-aminolevulinic acid) also carried out was in the same manner from 13C-labeled Na acetate. These were utilized in the study of the biosynthesis of chlorophyll and bacteriochlorophyll. L-[1-13C]glutamic acid-incorporated chlorophyll showed 13C-enriched peaks at sp3 region. This result shows that ring C atoms are derived from glutamic acid by the Beale route in Euglena gracilis. Incorporation of [2-13C]glycine by E. gracilis gave chlorophyll labeled at 10b Me ester (52.4 ppm). In the same way, L-[13CH3]methionine was incorporated and showed an enriched peak at 52.4 ppm. This indicates that glycine was metabolized into methionine and was incorporated into 1 side chain of chlorophyll in E. gracilis. [2-13C]glycine-incorporated bacteriochlorophyll showed 13C-enriched peaks at sp2 region. Also the feeding expt. with [5-13C]ALA into bacteriochlorophyll showed the same result, indicating that ALA is derived from glycine by the Shemin route in Rhodospeudomonas spheroides. Furthermore, a feeding expt. with 13C-labeled ALA in 50% D2O medium and of 13C, 2H-double-labeled ALA into bacteriochlorophyll showed .alpha., .beta. isotope-shifted peaks at ring

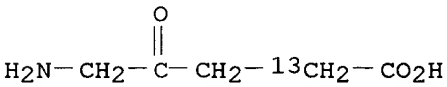
carbons. Thus, ring protons at the C5a, C3, C4, C8 position of bacteriochlorophyll are derived from water in R. spheroides.

IT **114791-06-9P 123253-92-9P 123253-93-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of and application to bacteriochlorophyll formation by Rhodospeudomonas spheroides)

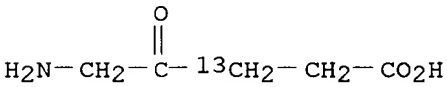
RN 114791-06-9 CAPLUS
CN Pentanoic-4-13C acid, 5-amino-4-oxo- (9CI) (CA INDEX NAME)



RN 123253-92-9 CAPLUS
CN Pentanoic-2-13C acid, 5-amino-4-oxo- (9CI) (CA INDEX NAME)



RN 123253-93-0 CAPLUS
CN Pentanoic-3-13C acid, 5-amino-4-oxo- (9CI) (CA INDEX NAME)

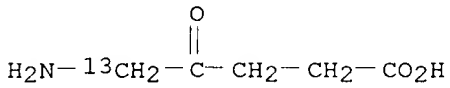


L16 ANSWER 20 OF 45 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1989:574621 CAPLUS
DOCUMENT NUMBER: 111:174621
TITLE: A facile synthesis of .delta.-aminolevulinic acid (ALA) regioselectively labeled with carbon-13 and direct observation of enzymatic transformation from ALA to porphobilinogen (PBG)
AUTHOR(S): Kurumaya, Katsuyuki; Okazaki, Takeo; Seido, Nobuo; Akasaka, Yuzuru; Kawajiri, Yoshiki; Kajiwara, Masahiro; Kondo, Masao
CORPORATE SOURCE: Meiji Coll. Pharm., Tanashi, 188, Japan
SOURCE: J. Labelled Compd. Radiopharm. (1989), 27(2), 217-35
CODEN: JLCRD4; ISSN: 0362-4803
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 111:174621

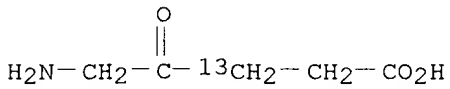
AB .delta.-Aminolevulinic acid (I) labeled with carbon-13 at position 1, 2, 3, 4, or 5, was synthesized from 13C-labeled glycine, Meldrum's acid, or bromoacetate. The latter compds. were prepd. from 13C-sodium acetate or 13C-acetic acid. Enzymic transformation of I to porphobilinogen was directly obsd. by 13C NMR.

IT **79503-87-0P 123253-93-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and enzymic transformation of, to porphobilinogen)

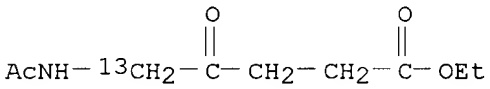
RN 79503-87-0 CAPLUS
CN Pentanoic-5-13C acid, 5-amino-4-oxo- (9CI) (CA INDEX NAME)



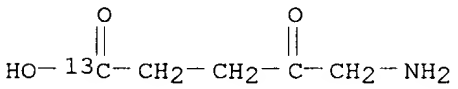
RN 123253-93-0 CAPLUS
CN Pentanoic-3-13C acid, 5-amino-4-oxo- (9CI) (CA INDEX NAME)



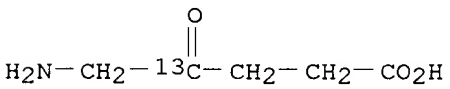
IT **113433-13-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hydrolysis or deuteration of)
RN 113433-13-9 CAPLUS
CN Pentanoic-5-13C acid, 5-(acetylamino)-4-oxo-, ethyl ester (9CI) (CA INDEX NAME)



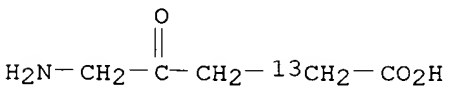
IT **98599-93-0P 114791-06-9P 123253-92-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 98599-93-0 CAPLUS
CN Pentanoic-1-13C acid, 5-amino-4-oxo- (9CI) (CA INDEX NAME)



RN 114791-06-9 CAPLUS
CN Pentanoic-4-13C acid, 5-amino-4-oxo- (9CI) (CA INDEX NAME)



RN 123253-92-9 CAPLUS
CN Pentanoic-2-13C acid, 5-amino-4-oxo- (9CI) (CA INDEX NAME)



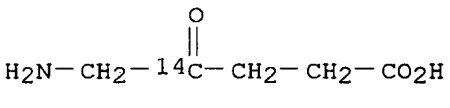
L16 ANSWER 21 OF 45 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1989:53854 CAPLUS
DOCUMENT NUMBER: 110:53854
Searched by Barb O'Bryen, STIC 308-4291

TITLE: Carbon-14 labeling and biological activity of the tumor-localizing derivative of hematoporphyrin
AUTHOR(S): Ho, Yau Kwan; Pandey, Ravindra K.; Missert, Joseph R.; Bellnier, David A.; Dougherty, Thomas J.
CORPORATE SOURCE: Oncol. Found. Buffalo, Buffalo, NY, 14203, USA
SOURCE: Photochem. Photobiol. (1988), 48(4), 445-9
CODEN: PHCBAP; ISSN: 0031-8655
DOCUMENT TYPE: Journal
LANGUAGE: English

AB 14C-labeled hematoporphyrin ([14C]HP) was synthesized by 2 methods. Using an in vitro avian whole-blood system, [14C]protoheme was obtained biosynthetically by incorporating [14C]aminolevulinic acid into the porphyrin ring structure. Subsequently, the [14C]protoheme was converted to [14C]HP by std. procedures. By adopting several well-characterized chem. reactions, deuteroporphyrin was treated with [14C]acetyl chloride, giving [14C]diacetyldeuteroporphyrin which was readily reduced and hydrolyzed to [14C]HP (with the 14C label on the hydroxyethyl side-chains). These 2 methods are simple and afford good yields of [14C]HP with moderate to high specific activities. The [14C]HP was then treated with AcOH/H2SO4 followed by NaOH to give [14C]HPD. Upon gel and ultrafiltration, the [14C]HPD was enriched in the so-called tumor-localizing fraction of HPD, giving [14C]Photofrin II (PII) with specific activities of 0.4 Ci/mol (biosynthesis) and 10 Ci/mol (chem. synthesis). These [14C]PII prepns. were equiv. with respect to chromatog. and spectrophotometric characteristics, as well as tumoricidal photodynamic activity in the DBA/2 Ha-DD mouse: SMT-F tumor system, to the unlabeled com. product Photofrin II. The distribution of [14C]PII in mouse tissues was in close agreement to that previously reported, after adjustment for dose, for [14C]HPD biosynthetically labeled in vivo, as well as for Photofrin II, where tissue levels were detd. spectrophotometrically after extn.

IT **7729-71-7**
RL: PROC (Process)
(incorporation of, into porphyrin)

RN 7729-71-7 CAPLUS
CN Pentanoic-4-14C acid, 5-amino-4-oxo- (9CI) (CA INDEX NAME)



L16 ANSWER 22 OF 45 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1988:611234 CAPLUS
DOCUMENT NUMBER: 109:211234
TITLE: Labeling method with enriched carbon-13 stable isotopes
AUTHOR(S): Kajiwara, Masahiro
CORPORATE SOURCE: Meiji Coll. Pharm., Tokyo, 154, Japan
SOURCE: Saishin Igaku (1987), 42(6), 1328-31
CODEN: SAIGAK; ISSN: 0370-8241
DOCUMENT TYPE: Journal; General Review
LANGUAGE: Japanese

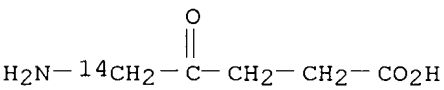
AB A review with 9 refs. on 13C-NMR as applied to the mol. structural study of natural products. Syntheses of [4-13C]-(2RS)-.alpha.-tocopherol and [4-13C]-(2RS)-.alpha.-tocopheryl acetate (I) were shown together with H noise-decoupled natural abundance 13C-FT NMR spectrum of DL-.alpha.-tocopheryl acetate and proton noise-decoupled 13C-FT NMR spectrum of 13C-enriched (I). Synthesis of [5-13C]-aminolevulinic acid (II) was shown with H noise-decoupled 13C-FT NMR spectrum of (II) and

[5-13C]-II. Biosynthesis of erythromycin A was shown with H noise-decoupled 13C-FT NMR spectrum of [1-13C]-sodium propionate enriched erythromycin A.

IT **5976-91-0P**
RL: PREP (Preparation)
(synthesis and carbon-13 NMR of)

RN 5976-91-0 CAPLUS

CN Pentanoic-5-14C acid, 5-amino-4-oxo- (9CI) (CA INDEX NAME)



L16 ANSWER 23 OF 45 CAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1988:419382 CAPLUS

DOCUMENT NUMBER: 109:19382

TITLE: Carbon-13 NMR studies of methylene and methine carbons of substrate bound to a 280,000-dalton protein, porphobilinogen synthase

AUTHOR(S): Jaffe, Eileen K.; Markham, George D.

CORPORATE SOURCE: Sch. Dent. Med., Univ. Pennsylvania, Philadelphia, PA, 19104-6002, USA

SOURCE: Biochemistry (1988), 27(12), 4475-81
CODEN: BICHAW; ISSN: 0006-2960

DOCUMENT TYPE: Journal

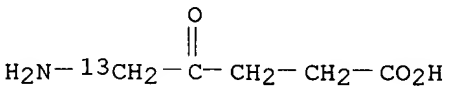
LANGUAGE: English

AB 13C NMR was used to observe the equil. complex of [5,5-2H,5-13C]-5-aminolevulinate ([5,5-2H,5-13C]ALA) bound to porphobilinogen (PBG) synthase (5-aminolevulinate dehydratase), a 280,000-dalton protein. [5,5-2H, 5-13C]ALA (chem. shift 46.9 ppm in D2O) was prepd. from [5-13C]ALA through enolization in deuteriated neutral potassium phosphate buffer. In the PBG synthase reaction [5,5-2H,5-13C]ALA forms [2,11,11-2H,2,11-13C]PBG (chem. shifts 116.2 ppm for C2 and 34.2 ppm for C11 in D2O). For the complex formed between [5,5-2H,5-13C]ALA and Me methanethiosulfonate (MMTS)-modified PBG synthase, which does not catalyze PBG formation but can form a Schiff base adduct, the chem. shift of 44.2 ppm (line width 92 Hz) identified an imine structure as the predominant tautomeric form of the Schiff base. By comparison to model compds., the stereochem. of the imine was deduced; however, the protonation state of the imine atom remained unresolved. Reconstitution of the MMTS-modified enzyme-Schiff base complex with Zn(II) and 2-mercaptoethanol resulted in the holoenzyme-bound equil. complex; this complex contained predominantly enzyme-bound PBG, and spectra revealed 2 peaks from bound PBG and 2 from free PBG. For bound PBG, C2 was -2.8 ppm from the free signal and C11 was +2.6 ppm from the free signal; the line widths of the bound signals were 55 and 75 Hz, resp. To aid in interpretation of these shifts, and those previously obsd. with [4-13C]ALA as substrate (which forms [3,5-13C]PBG), the 13C NMR chem. shifts of PBG were investigated as functions of pH and a variety of org. solvents. The obsd. shifts of bound PBG were not consistent with simple protonation/deprotonation of PBG nor with changes that could be duplicated by solvation by simple org. solvents.

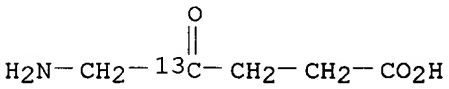
IT **79503-87-0**
RL: BIOL (Biological study)
(deuteriation of)

RN 79503-87-0 CAPLUS

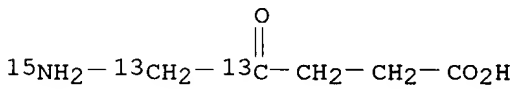
CN Pentanoic-5-13C acid, 5-amino-4-oxo- (9CI) (CA INDEX NAME)



IT **114791-06-9**
RL: RCT (Reactant)
(reaction of, with porphobilinogen synthase)
RN 114791-06-9 CAPLUS
CN Pentanoic-4-13C acid, 5-amino-4-oxo- (9CI) (CA INDEX NAME)



L16 ANSWER 24 OF 45 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1988:150138 CAPLUS
DOCUMENT NUMBER: 108:150138
TITLE: A new synthesis and NMR-spectroscopy of [15N-5,4-13C]-aminolevulinic acid
AUTHOR(S): Nitsche, Bernhard; Koest, Hans Peter; Cmiel, Edmund; Schneider, Siegfried
CORPORATE SOURCE: Inst. Phys. Theor. Chem., Tech. Univ. Muenchen, Garching, D-8046, Fed. Rep. Ger.
SOURCE: J. Labelled Compd. Radiopharm. (1987), 24(6), 623-30
CODEN: JLCRD4; ISSN: 0362-4803
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 108:150138
AB H215N13CH213COCH2CH2CO2H was prepd. from 13C.
IT **113639-01-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 113639-01-3 CAPLUS
CN Pentanoic-4,5-13C2 acid, 5-(amino-15N)-4-oxo-, hydrochloride (9CI) (CA INDEX NAME)



L16 ANSWER 25 OF 45 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1988:131031 CAPLUS
DOCUMENT NUMBER: 108:131031
TITLE: Preparation of 13C-labeled aminolevulinic acid as a pharmaceutical intermediate
INVENTOR(S): Kajiwara, Masahiro
PATENT ASSIGNEE(S): Japan Spectroscopic Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
Searched by Barb O'Bryen, STIC 308-4291

LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

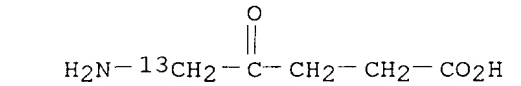
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 62111954	A2	19870522	JP 1985-251070	19851109

AB Stable 13C-labeled aminolevulinic acid (I), useful as a pharmaceutical intermediate, is prepd. from a 13C-labeled nitrile compd. A mixt. of 3-carbethoxypropionyl chloride and Cu13CN in MeCN was refluxed at 100.degree. in Ar to give EtO2CCH2CH2CO13CN which was treated with Zn powder in AcOH-Ac2O at 40.degree. under ultrasound to give 98% EtO2CCHCH2CO13CH2NHAc which was hydrolyzed to give I having >90% 5-13C.

IT **79503-87-0P**, Aminolevulinic acid (5-13C)
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn of, as pharmaceutical intermediate)

RN 79503-87-0 CAPLUS

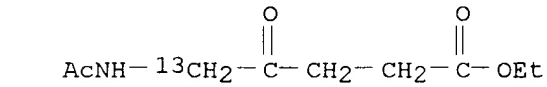
CN Pentanoic-5-13C acid, 5-amino-4-oxo- (9CI) (CA INDEX NAME)



IT **113433-13-9P**, N-Ethyl-4-keto-5-13C-aminoacetopentanoate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hydrolysis of)

RN 113433-13-9 CAPLUS

CN Pentanoic-5-13C acid, 5-(acetylamino)-4-oxo-, ethyl ester (9CI) (CA INDEX NAME)



L16 ANSWER 26 OF 45 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1988:90998 CAPLUS
DOCUMENT NUMBER: 108:90998
TITLE: The preparation of radiolabeled porphyrins and their use in studies of photodynamic therapy
AUTHOR(S): Vernon, David I.; Brown, Stanley B.
CORPORATE SOURCE: Dep. Biochem., Univ. Leeds, Leeds, LS2 9JT, UK
SOURCE: Photochem. Photobiol. (1987), 46(5), 581-6
CODEN: PHCBAP; ISSN: 0031-8655
DOCUMENT TYPE: Journal
LANGUAGE: English

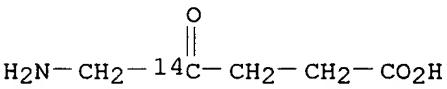
AB The use of radiolabeled HPD and DHE has potential importance in studies of the mechanism of localization of these compds. in tumors and their mode of action in promoting light-mediated cell damage. A no. of methods of prepn. of radiolabeled HPD and its components have been investigated. In a novel approach, methods were developed for producing 14C- or 3H-labeled protoporphyrin from photosynthetic algae. In this way, hematoporphyrin and HPD can be produced with much higher specific radioactivity than has hitherto been available. This radiolabeled material has been used in several studies related to photodynamic therapy. One application has been the precise detn. of the molar absorption coeff. of DHE (and other components of HPD) based on the fact that its specific radioactivity per porphyrin unit must be identical to that of the porphyrin from which it

was prepd.

IT **7729-71-7**, 5-Amino[4-14C]levulinic acid
RL: BIOL (Biological study)
(in carbon-14-labeled protoporphyrin IX and protoheme prepn.)

RN 7729-71-7 CAPLUS

CN Pentanoic-4-14C acid, 5-amino-4-oxo- (9CI) (CA INDEX NAME)



L16 ANSWER 27 OF 45 CAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1988:6363 CAPLUS

DOCUMENT NUMBER: 108:6363

TITLE: Synthesis of selectively multi-labeled histidine with stable isotopes for study of histidinaemia by GLC-mass spectrometry

AUTHOR(S): Furuta, Takashi; Kasuya, Yasuji; Takahashi, Hidenori; Baba, Shigeo

CORPORATE SOURCE: Dep. Clin. Pharm., Tokyo Coll. Pharm., Hachioji, 192-03, Japan

SOURCE: J. Chem. Res., Synop. (1987), (3), 86-7
CODEN: JRPSDC; ISSN: 0308-2342

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 108:6363

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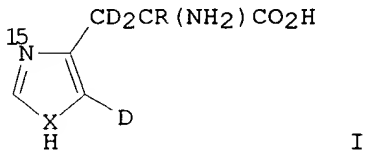


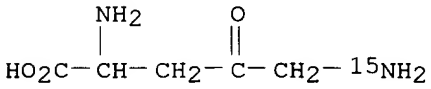
I

AB Labeled histidines L-I (X = N, R = H) and DL-I (X = 15N, R = D) were prepd from 2,5-diamino-4-oxopentanoic acid for use as biol. and anal. internal stds.

IT **111652-34-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and deuteration of)

RN 111652-34-7 CAPLUS

CN Ornithine-N5-15N, 4-oxo- (9CI) (CA INDEX NAME)



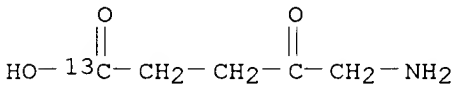
L16 ANSWER 28 OF 45 CAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1987:81332 CAPLUS

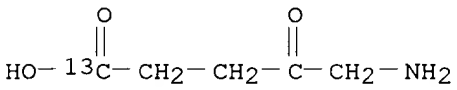
DOCUMENT NUMBER: 106:81332

TITLE: Mechanistic studies on the phytylation and methylation

steps in bacteriochlorophyll a biosynthesis: an application of the oxygen-18-induced isotope effect in carbon-13 NMR
AUTHOR(S): Emery, Vincent C.; Akhtar, Muhammad
CORPORATE SOURCE: Dep. Biochem., Univ. Southampton, Southampton, SO9 3TU, UK
SOURCE: Biochemistry (1987), 26(4), 1200-8
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The high-resoln. 13C NMR spectrum of bacteriochlorophyll a biosynthesized from [1-13C,1,1,4-18O3]-5-aminolevulinic acid by growing cells of Rhodopseudomonas sphaeroides has shown both the C-173 and C-133 resonances consist of 3 addnl. components upfield shifted from the 16O-13C:16O resonance. By comparison with the 13C NMR spectrum obtained for phytyl acetate contg. 13C and 18O selectively in the ester linkage, these components have been identified as the bridge (-18O-13C:16O), nonbridge (-16O-13C:18O), and dual-labeled (-18O-13c:18O) isotopomers. These results suggest that both the ester bonds of bacteriochlorophyll a are produced by a carboxy-alkyl transfer process.
IT **98599-93-0P 106213-17-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction of)
RN 98599-93-0 CAPLUS
CN Pentanoic-1-13C acid, 5-amino-4-oxo- (9CI) (CA INDEX NAME)

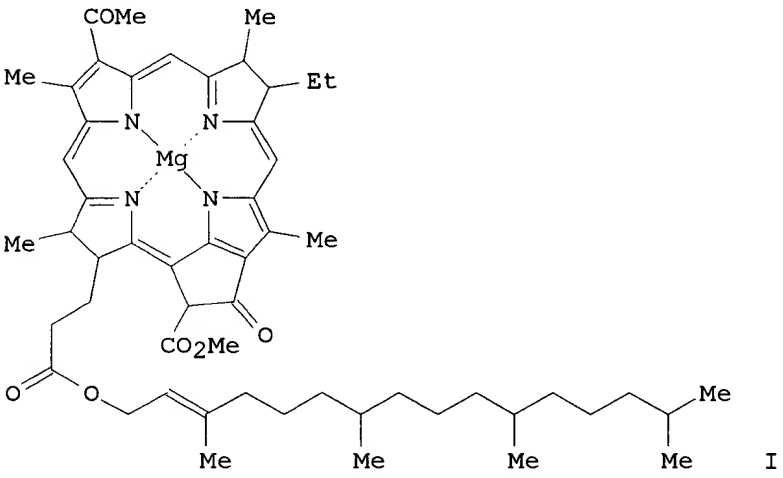


RN 106213-17-6 CAPLUS
CN Pentanoic-1-13C acid, 5-amino-4-oxo-, hydrochloride (9CI) (CA INDEX NAME)



L16 ANSWER 29 OF 45 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1985:557030 CAPLUS
DOCUMENT NUMBER: 103:157030
TITLE: Mechanistic studies on the phytylation step in bacteriochlorophyll a biosynthesis: an application of the oxygen-18 induced isotope effect in carbon-13 NMR spectroscopy
AUTHOR(S): Emery, Vincent C.; Akhtar, Muhammad
CORPORATE SOURCE: Dep. Chem., Univ. Southampton, Southampton, SO9 3TU, UK
SOURCE: J. Chem. Soc., Chem. Commun. (1985), (9), 600-1
CODEN: JCCCAT; ISSN: 0022-4936
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

Searched by Barb O'Bryen, STIC 308-4291

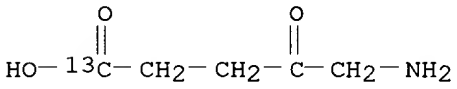


AB A 13C NMR spectral study showed that bacteriochlorophyll a (I) formed from H2NCH2C18O(CH2)213C18O2H (.delta.-aminolevulinic acid) in cultures of Rhodopseudomonas sphaeroides at 27.degree. contained 18O in both the bridge and nonbridge O of the phytyl ester linkage. These results are in accord with the previously proposed phytylation mechanism in the biosynthesis of I (M. Akhtar, et al., 1980, 1984).

IT **98599-93-0**
RL: BIOL (Biological study)
(oxygen-18 labeling of)

RN 98599-93-0 CAPLUS

CN Pentanoic-1-13C acid, 5-amino-4-oxo- (9CI) (CA INDEX NAME)



L16 ANSWER 30 OF 45 CAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1983:157372 CAPLUS

DOCUMENT NUMBER: 98:157372

TITLE: A novel method for continuous monitoring of bilirubin production in unstressed rats

AUTHOR(S): Reichen, Juerg; Hoilien, Catherine; Sheldon, George F.; Kirshenbaum, Gerald

CORPORATE SOURCE: Sch. Med., Univ. Colorado, Denver, CO, 90262, USA

SOURCE: Am. J. Physiol. (1983), 244(3), G336-G340
CODEN: AJPHAP; ISSN: 0002-9513

DOCUMENT TYPE: Journal

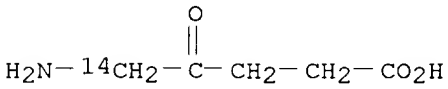
LANGUAGE: English

AB A device is described for continuous infusion and monitoring of exhaled 14CO as a test of hepatic bilirubin prodn. in rats. A Silastic catheter, implanted into a jugular vein under light ether anesthesia, was protected with a spring shield and a cannula swivel. The animals were kept in a modified Bollman cage. .delta.-[5-14C]aminolevulinic acid, a heme precursor yielding 14CO upon breakdown of heme to bilirubin, was infused at a const. rate. Exhaled 14CO was oxidized to 14CO2 and collected in ethanolamine. The efficiency of the system averaged 97.8%. In untreated

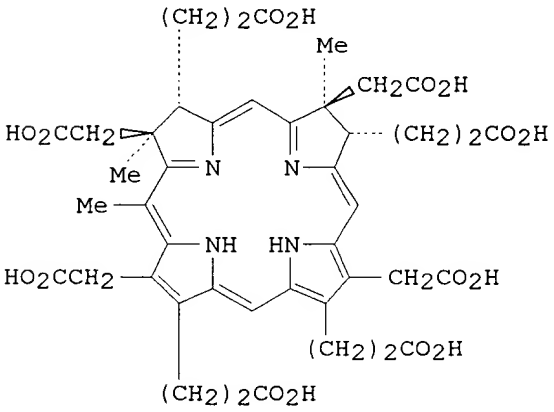
animals, 14CO prodn. reached a plateau within 12 h; thereafter, it increased by 2.8%/day. The responsiveness of the system was tested by fasting the animals, which stimulated hepatic bilirubin prodn. Fasting increased 14CO prodn. by 32.8% (mean) after 72 h. This was assocd. with an increase in hepatic heme oxygenase activity (+45%) and a decrease in microsomal cytochrome P 450 content (-45%). The approach permits continuous monitoring of hepatic bilirubin prodn. without subjecting the animals to the stress of handling, restraint, or anesthesia. The method can easily be applied to other breath tests involving formation of 14CO2.

IT **5976-91-0**
RL: ANST (Analytical study)
(in bilirubin formation by liver anal.)

RN 5976-91-0 CAPLUS
CN Pentanoic-5-14C acid, 5-amino-4-oxo- (9CI) (CA INDEX NAME)



L16 ANSWER 31 OF 45 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1981:585521 CAPLUS
DOCUMENT NUMBER: 95:185521
TITLE: The structure of factor III. A trimethyl isobacteriochlorin intermediate in the biosynthesis of vitamin B12
AUTHOR(S): Mueller, Gerhard; Gneuss, K. D.; Kriemler, H. P.; Irwin, Anthony J.; Scott, A. I.
CORPORATE SOURCE: Inst. Org. Chem. Biochem. Isotopenforsch., Univ. Stuttgart, Stuttgart, D-7000/1, Fed. Rep. Ger.
SOURCE: Tetrahedron, Suppl. (1981), (9), 81-90
CODEN: TETSAE; ISSN: 0563-2072
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



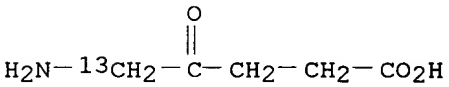
I

AB The structure of Factor III, an intermediate in corrin formation in Propionibacterium shermanii, was detd. by 13C and 1H NMR anal. of a 13C-enriched sample to be I rather than a C-5 methylated

isobacteriochlorin as previously reported of (Batterby, A. R.; et al., 1977, 1978). In cell-free exts. of Clostridium tetanomorphum the conversion of Factor III to cobyrinic acid involves loss of C-20 together with the methionine-derived Me group attached in this position. The observations are discussed with ref. to the connection between urogen and corrin biosynthesis.

IT **79503-87-0**
RL: RCT (Reactant)
(microbial reaction of, with labeled methionine, methylsirohydrochlorin by)

RN 79503-87-0 CAPLUS
CN Pentanoic-5-13C acid, 5-amino-4-oxo- (9CI) (CA INDEX NAME)

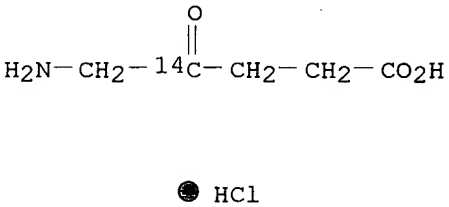


L16 ANSWER 32 OF 45 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1981:480056 CAPLUS
DOCUMENT NUMBER: 95:80056
TITLE: Synthesis of carbon-14-labeled 5-hydroxy-4-ketovaleric acid and 4,5-dioxovaleric acid
AUTHOR(S): Tschesche, Rudolf; Wirth, Wolfgang
CORPORATE SOURCE: Inst. Org. Chem. Biochem., Univ. Bonn, Bonn, D-5300/1, Fed. Rep. Ger.
SOURCE: J. Labelled Compd. Radiopharm. (1981), 18(3), 433-8
CODEN: JLCRD4; ISSN: 0362-4803
DOCUMENT TYPE: Journal
LANGUAGE: English

AB HOCH2CO(CH2)214CO2H (I) was prepd. by Grignard reaction of 1-benzyloxy-4-bromo-2-butanone ethylene acetal with 14CO2 and subsequent removal of the protecting groups. Deamination of H2NCH214CO(CH2)2CO2H.HCl by HNO2 gave HOCH214CO(CH2)2CO2H. Oxidn. of I [Cu(OAc)2, H2O, under N, room temp., 3 days) gave the corresponding 4,5-dioxovaleric acid.

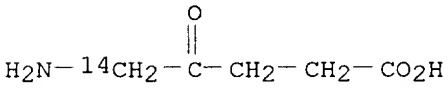
IT **16387-80-7**
RL: RCT (Reactant)
(deamination of)

RN 16387-80-7 CAPLUS
CN Pentanoic-4-14C acid, 5-amino-4-oxo-, hydrochloride (9CI) (CA INDEX NAME)

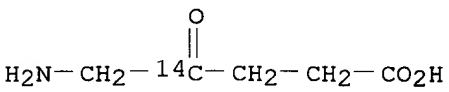


L16 ANSWER 33 OF 45 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1980:211263 CAPLUS
DOCUMENT NUMBER: 92:211263
TITLE: Investigation of a non-invasive method for measuring metabolic changes in obesity
AUTHOR(S): Vineyard, Michelle L.; Smith, John T.
CORPORATE SOURCE: Dep. Food Sci. Nutr. Food Syst. Adm., Univ. Tennessee, Knoxville, TN, USA
Searched by Barb O'Bryen, STIC 308-4291

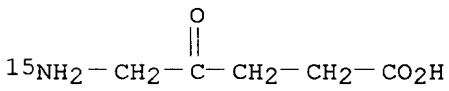
SOURCE: Tenn. Farm Home Sci., Prog. Rep. (1979), 112, 29-30
CODEN: TFHSAT; ISSN: 0040-3229
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A method is described for measuring 14CO excretion following administration of .delta.-aminolevulinic-5-14C acid in obese mice. Since .delta.-aminolevulinic acid is a precursor for hemoprotein synthesis, esp. cytochrome P 450, the excretion of 14CO serves as an indicator of the activity of the hepatic mixed function oxidase system, which may be involved in obesity. Excreted 14CO was collected by a closed circulation system, oxidized to 14CO2 by PdCl2, and the radioactivity counted. When Na pentobarbital, which causes an increase in cytochrome P 450, was administered, there was a large increase in 14CO excretion when the induction was for 3-6 days. Moreover, the obese mice excreted 26% less 14CO than the controls at 3-4 mo of age, and 47% less 14CO at 6-8 mo. Thus, the administration of .delta.-aminoleuvulinic-5-14C acid and collection of 14CO indicated that obese mice had less cytochrome P 450.
IT **5976-91-0**
RL: ANST (Analytical study)
(in metabolic studies of obesity)
RN 5976-91-0 CAPLUS
CN Pentanoic-5-14C acid, 5-amino-4-oxo- (9CI) (CA INDEX NAME)



L16 ANSWER 34 OF 45 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1978:503111 CAPLUS
DOCUMENT NUMBER: 89:103111
TITLE: A rapid, simple method for obtaining radiochemically pure hepatic heme
AUTHOR(S): Bonkowsky, Herbert Lloyd; Bement, William Jay; Erny, Raymond
CORPORATE SOURCE: Hepatol. Metab. Lab., VA Cent., White River Junction, Vt., USA
SOURCE: Biochim. Biophys. Acta (1978), 541(1), 119-23
CODEN: BBACAQ; ISSN: 0006-3002
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A simple, rapid method for obtaining radiochem. pure heme synthesized in vivo in rat liver from .delta.-aminolevulinate-4-14C has been devised, by modifying the procedure of H. L. Bonkowksy, et al. (1975). This method, in which the heme is extd. into EtOAc/AcOH and in which porphyrins are removed from the heme-contg. org. phase with HCl washes, does not require addn. of carrier heme. The new method gives heme recoveries better than and heme sp. activities identical to those obtained using the crystn. method. In this new method heme must be synthesized from .delta.-aminolevulinate-4-14C; it not satisfactory to use glycine-2-14C substrate because nonheme counts are isolated in the heme fraction.
IT **7729-71-7**
RL: ANST (Analytical study)
(carbon-14-labeled heme formation from, in liver, sepn. after)
RN 7729-71-7 CAPLUS
CN Pentanoic-4-14C acid, 5-amino-4-oxo- (9CI) (CA INDEX NAME)



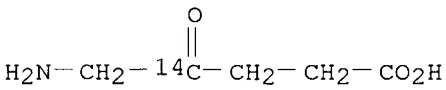
L16 ANSWER 35 OF 45 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1976:521317 CAPLUS
DOCUMENT NUMBER: 85:121317
TITLE: Quantitation of ineffective erythropoiesis from the incorporation of [15N]delta-aminolevulinic acid and [15N]-glycine into early labeled bilirubin
AUTHOR(S): Samson, Diana; Halliday, D.; Nicholson, D. C.; Chanarin, I.
CORPORATE SOURCE: MRC Clin. Res. Cent., Northwick Park Hosp., Harrow/Middlesex, Engl.
SOURCE: Br. J. Haematol. (1976), 34(1), 33-44
CODEN: BJHEAL
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The incorporation of glycine-15N into early labeled bilirubin and Hb heme was measured in 4 hematol. normal subjects, using the clearance of bilirubin-14C to measure total bilirubin prodn. rate. Hepatic heme turnover was calcd. from the incorporation of .delta.-aminolevulinic-15N acid into early labeled bilirubin. From the exptl. data and previously published data in normal subjects a method is derived for the quantitation of ineffective erythropoiesis which can be applied to similar studies in patients with hematol. disorders.
IT **60556-69-6**
RL: BIOL (Biological study)
(in erythropoiesis detn.)
RN 60556-69-6 CAPLUS
CN Pentanoic acid, 5-(amino-15N)-4-oxo- (9CI) (CA INDEX NAME)



L16 ANSWER 36 OF 45 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1975:602810 CAPLUS
DOCUMENT NUMBER: 83:202810
TITLE: Formation of cobyrinic acid by means of a cell-free system from Clostridium tetanomorphum. Comparative examinations with carbon-14-labeled 5-aminolevulinate and carbon-14-labeled uroporphyrinogen
AUTHOR(S): Dauner, Hans O.; Mueller, Gerhard
CORPORATE SOURCE: Inst. Org. Chem., Biochem. Isotopenforsc, Univ. Stuttgart, Stuttgart, Ger.
SOURCE: Hoppe-Seyler's Z. Physiol. Chem. (1975), 356(9), 1353-8
CODEN: HSZPAZ
DOCUMENT TYPE: Journal
LANGUAGE: German
AB Cell-free exts. from C. tetanomorphum, a microorganism which synthesizes corrins but no heme, converted both 5-aminolevulinate and uroporphyrinogen III into cobyrinic acid. Comparative examns. with 5-aminolevulinate-14C and uroporphyrinogen-14C yielded corresponding results. Cell-free exts. from C. tetanomorphum contained uroporphyrinogen III. To obtain good

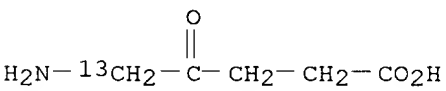
radiochem. yields it was therefore necessary to use substrates of high-specific radioactivity. A method for the prepn. of 14C-labeled uroporphyrin I-IV with high specific radioactivity is described.

IT **16387-80-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 16387-80-7 CAPLUS
CN Pentanoic-4-14C acid, 5-amino-4-oxo-, hydrochloride (9CI) (CA INDEX NAME)



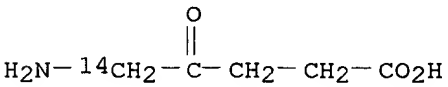
L16 ANSWER 37 OF 45 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1974:108498 CAPLUS
DOCUMENT NUMBER: 80:108498
TITLE: Biosynthesis of porphyrins and related macrocycles. II. Synthesis of .delta.-amino[5-13C]levulinic acid and [11-13C]porphobilinogen. Incorporation of the latter into protoporphysin IX
AUTHOR(S): Battersby, Alan R.; Hunt, Eric; McDonald, Edward; Moron, Jaqueline
CORPORATE SOURCE: Univ. Chem. Lab., Cambridge, Engl.
SOURCE: J. Chem. Soc., Perkin Trans. 1 (1973), (23), 2917-22
CODEN: JCPRB4
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB H2N13CH2CO(CH2)2CO2H.HCl and [11-13C]porphobilinogen lactam (I) were prepd. in 57 and 43% overall yield from OCH(CH2)2CO2Et and the methyl pyrrole (II, R = H, R1 = Et, R2 = CO2Et), resp. Hydrolysis of I gave II (R = NH2, R1 = R2 = H) incorporation of which into protoporphyrin IX by Euglena gracilis gave a product equally labeled at the meso-C atoms.

IT **52065-79-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 52065-79-9 CAPLUS
CN Pentanoic-5-13C acid, 5-amino-4-oxo-, hydrochloride (9CI) (CA INDEX NAME)

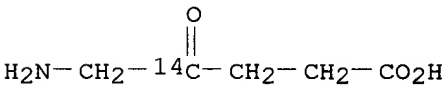


L16 ANSWER 38 OF 45 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1973:526756 CAPLUS
DOCUMENT NUMBER: 79:126756
TITLE: Carbon-14 labeled amino acids, amino keto acids, and amino ketones of interest in biology
Searched by Barb O'Bryen, STIC 308-4291

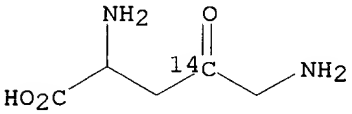
AUTHOR(S): Beaucourt, J. P.
CORPORATE SOURCE: Univ. Paris, Orsay, Fr.
SOURCE: Report (1972), FRNC-TH-322, 274 pp. Avail.: Dep. NTIS (U. S. Sales Only)
From: Nucl. Sci. Abstr. 1973, 28(3), 5274
DOCUMENT TYPE: Report
LANGUAGE: French
AB Four methods of synthesizing 4-14C- or 5-14C-.delta.-aminolevulinic acid as well as the prepn. of 4-14C-homoserine, 4-14C-methionine, 4-14C-.gamma.-butyrolactone, 7-14C-adrenalone, 4-14C-4-ketoornithine, and 14C-labeled keto esters, amino ketones, ketones, and keto acids were described.
IT **5976-91-0P 7729-71-7P 43189-68-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 5976-91-0 CAPLUS
CN Pentanoic-5-14C acid, 5-amino-4-oxo- (9CI) (CA INDEX NAME)



RN 7729-71-7 CAPLUS
CN Pentanoic-4-14C acid, 5-amino-4-oxo- (9CI) (CA INDEX NAME)



RN 43189-68-0 CAPLUS
CN Ornithine-4-14C, 4-oxo- (9CI) (CA INDEX NAME)



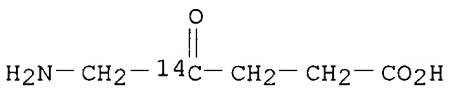
L16 ANSWER 39 OF 45 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1973:94541 CAPLUS
DOCUMENT NUMBER: 78:94541
TITLE: Method for the biological preparation and thin-layer chromatographic purification of [14C]-protochlorophyllide a
AUTHOR(S): Ellsworth, R. K.; Nowak, C. A.
CORPORATE SOURCE: Coll. Arts Sci., State Univ. New York, Plattsburgh, N. Y., USA
SOURCE: Anal. Biochem. (1973), 51(2), 656-62
CODEN: ANBCA2
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A method is described for the synthesis of protochlorophyllide-14C (I) in wheat seedlings (Triticum aestivum) and purifn. by a 2-step thin-layer chromatog. procedure. Seeds were germinated in vermiculite and grown for 5 days at 24.degree. in darkness. Seedlings were then grown for 5 days in a 0.02M phosphate buffer, at pH 7.7, contg. .delta.-aminolevulinic

acid-4-14C (II) (sp. activity 18.3 .mu.Ci/.mu.mole). The 10-day old etiolated seedlings were then macerated and extd. The Metalloporphyrins-14C were extd. and a crude ext. carrier of I, obtained from a parallel wheat not exposed to II, was added. Purifn. of crude I to radiochem. and spectrometric homogeneity was accomplished in 2 steps: thin-layer chromatog. on silica gel G plates and extn. of the eluate with Me2CO and Et2O. The 2nd purifn. step was done on sucrose thin-layer plates, scraping the bands directly into Et2O.

IT **7729-71-7**
RL: ANST (Analytical study)
(in protochlorophyllide a prepn.)

RN 7729-71-7 CAPLUS

CN Pentanoic-4-14C acid, 5-amino-4-oxo- (9CI) (CA INDEX NAME)



L16 ANSWER 40 OF 45 CAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1972:113498 CAPLUS

DOCUMENT NUMBER: 76:113498

TITLE: New methods of synthesis of .delta.-aminolevulinic acid-4-14C and -5-14C/.delta.-aminolevulinic acid-4-14C or -5-14C

AUTHOR(S): Pichat, L.; Beaucourt, J. P.; Herbert, M.

CORPORATE SOURCE: C.E.N., Saclay, Fr.

SOURCE: Radioisotopy (1971), 12(4), 519-34
CODEN: RAISBC

DOCUMENT TYPE: Journal

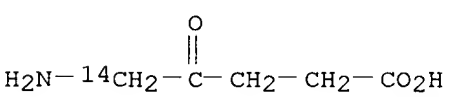
LANGUAGE: English

AB Shorter and more efficient methods of prepn. of .delta.-aminolevulinic acid (I) are proposed. The first method starts from glycine-[1-14C]. Phthalylglycyl chloride is condensed at 0.degree. in ether and 1,2-dimethoxyethane with a lithium deriv. made from BuLi and tris(trimethylsilyl) 1,1,2-ethanetricarboxylate. After hydrolysis of the nonisolated intermediate, and two chromatographic purifications the overall yield of pure I-[4-14C] is 60%. When applied to glycine-[2-14C] the method provides I-[5-14C]. It is also shown to be a general method of prepn. of .gamma.-, .delta.-, .epsilon.-oxo acids and methyl ketones. The second method is based on carbonation with 14CO2 of the Grignard reagent where the potential carboxyl group is protected as 2,4,10-trioxaadamantane, to give the half ortho succinic ester. The latter is then transformed into the corresponding chloride which is treated by the Arndt-Eistert method in order to provide the bromo ketone. After phthalimidation, the intermediate is hydrolyzed to I-[4-14C]. The overall yield based on 14CO2 is 30%. Self-decompn. rates under various storage conditions are tabulated for I-[4-14C] and -[2,3-T].

IT **5976-91-0P 7729-71-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

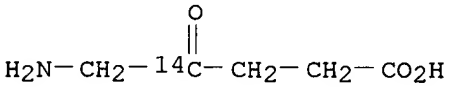
RN 5976-91-0 CAPLUS

CN Pentanoic-5-14C acid, 5-amino-4-oxo- (9CI) (CA INDEX NAME)

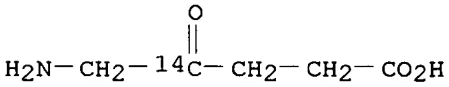


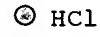
Searched by Barb O'Bryen, STIC 308-4291

RN 7729-71-7 CAPLUS
CN Pentanoic-4-14C acid, 5-amino-4-oxo- (9CI) (CA INDEX NAME)



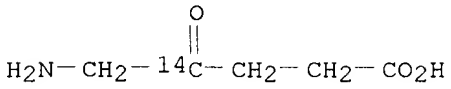
IT **16387-80-7**
RL: PRP (Properties)
(stability of)
RN 16387-80-7 CAPLUS
CN Pentanoic-4-14C acid, 5-amino-4-oxo-, hydrochloride (9CI) (CA INDEX NAME)



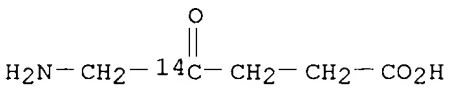


L16 ANSWER 41 OF 45 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1968:95278 CAPLUS
DOCUMENT NUMBER: 68:95278
TITLE: Synthesis of .delta.-aminolevulinic acid. Application to the introduction of carbon-14 and of tritium
AUTHOR(S): Loheac, Joel
CORPORATE SOURCE: C. E. N., Saclay, Fr.
SOURCE: Commis. Energ. At. [Fr.], Rapp. (1967), No. CEA-R 3063, 84 pp.
CODEN: CMEAAQ
DOCUMENT TYPE: Journal
LANGUAGE: French
GI For diagram(s), see printed CA Issue.
AB Incorporation of 14C and T into .delta.-aminolevulinic acid HO2CCH2CH2COCH2NH2 (I) was considered of special interest due to the biol. importance of the compd. Special effort was devoted to the incorporation of 14C into position 4 of I, because this C-atom participates in the formation of pyrrole rings and protoporphyrin. The method produced a yield of 30% and consisted of the following steps: carboxylation using 14C of BrMgCH2CH2CH:CH2 produced allyl-acetic acid. Using ClCOCOCl the acid chloride was obtained which with CH2N2 and HCl produced ClCH214COCH2CH2CH:CH2 which was condensed with K phthalimide in dimethyl-formamide. The resulting II was oxidized and hydrolyzed to I. For the incorporation of 14C into positions 1 and 2, phthalimidoacetylacetate was treated with BrCH214CO2H in CH2N2. Acid hydrolysis produced 14C in position 1 of I but not in position 2. Incorporation of T into positions 2 and 3 succeeded. To avoid exchange reactions during tritiation of I which would lead to products with labile T and no biol. significance, Me .delta.-phthalimidodehydrolevulate (III, R = Me) was used. This compd. was produced either by the Wittig reaction or from furfurylamine according to the method of Marei and Raphael and modified by Sparatore and Cuming. Omitting hydrogenation, a hitherto unknown compd., .delta.-phthalimidodehydrolevulinic acid (III, R = H) was obtained, which after hydrolysis with HCl produced I. 70 references.
IT **7729-71-7P**

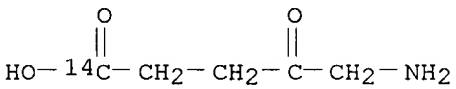
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 7729-71-7 CAPLUS
CN Pentanoic-4-14C acid, 5-amino-4-oxo- (9CI) (CA INDEX NAME)



L16 ANSWER 42 OF 45 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1968:94983 CAPLUS
DOCUMENT NUMBER: 68:94983
TITLE: Preparation of carbon-14-labeled molecules. VII. Synthesis of .delta.-aminolevulinic acid labeled with carbon-14 and tritium
AUTHOR(S): Herbert, Michel; Pichat, Louis
SOURCE: Bull. Inf. Sci. Tech., Commis. Energ. At. (Fr.) (1967), No. 118, 42-4
CODEN: BUIAAN
DOCUMENT TYPE: Journal
LANGUAGE: French
AB Various methods of labeling .gamma.-aminolevulinic acid with 14C, 3H, and 15N are described.
IT **7729-71-7P 13855-42-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 7729-71-7 CAPLUS
CN Pentanoic-4-14C acid, 5-amino-4-oxo- (9CI) (CA INDEX NAME)



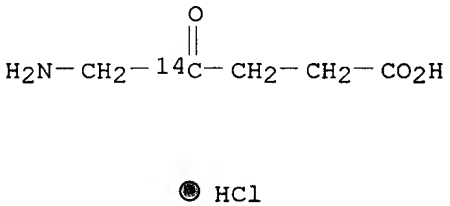
RN 13855-42-0 CAPLUS
CN Levulinic-1-14C acid, 5-amino- (8CI) (CA INDEX NAME)

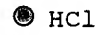


L16 ANSWER 43 OF 45 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1967:443377 CAPLUS
DOCUMENT NUMBER: 67:43377
TITLE: Improvement in the method of synthesis of .delta.-amino-levulinic acid-4-14C hydrochloride
AUTHOR(S): Mitta, Aldo E. A.; Ferramola, A. M.; Sancovich, H. A.; Grinstein, Moises
CORPORATE SOURCE: Com. Nacl. Energia At., Buenos Aires, Argent.
SOURCE: J. Labelled Compd. (1967), 3(1), 20-3
CODEN: JLCAAI
DOCUMENT TYPE: Journal
LANGUAGE: English
AB .delta.-Aminolevulinic acid-4-14C was prepd. from phthalimide using K14CN as the radioactive starting material. This method avoids the less

practical synthesis via glycine-14C and its condensation with phthalic anhydride to afford phthalylglycine-1-14C whose yield, based on K14CN, is thus considerably improved. 15 references.

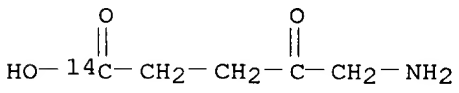
IT **16387-80-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 16387-80-7 CAPLUS
CN Pentanoic-4-14C acid, 5-amino-4-oxo-, hydrochloride (9CI) (CA INDEX NAME)



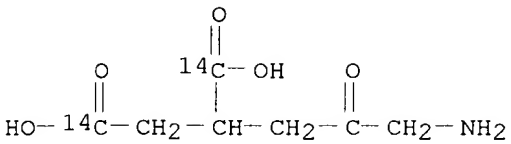


L16 ANSWER 44 OF 45 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1967:65013 CAPLUS
DOCUMENT NUMBER: 66:65013
TITLE: New methods of synthesis of 14C and tritium labeled .delta.-aminolevulinic acid. II. .delta.-Aminolevulinic -1-14C or -2-14C acid from sodium acetate-2-14C or -1-14C and ethyl phthalimidoacetyl acetate
AUTHOR(S): Pichat, Louis; Loheac, Joel; Herbert, Michel; Chatelain, G.
CORPORATE SOURCE: Serv. Mol. Marquees, C.E.N., Saclay, Fr.
SOURCE: Bull. Soc. Chim. Fr. (1966), (10), 3271-3
CODEN: BSCFAS
DOCUMENT TYPE: Journal
LANGUAGE: French
GI For diagram(s), see printed CA Issue.
AB cf. CA 66, 54979g. Treatment of Et (phthalimidoacetyl)acetylacetate (Ia) with NH4OH in EtOH gave Et phthalimidoacetylacetate (I), m. 111-12.degree. (95% EtOH). NaOAc-1-14C was converted to bromoacetic acid and then, with CH2N2 in 1,2-dimethoxyethane, to Me bromoacetate-1-14C (II). I and II were condensed using NaH in 1,2-dimethoxyethane and the product hydrolyzed to give crude .delta.-aminolevulinic 1-14C acid. The yield from NaOAc was 55%. A secondary product (15%) obtained was shown to be 3-(2-aminoacetyl)pentane-1,5-dioic acid which was probably formed by the reaction of 2-mols. of II with the di-Na deriv. of I.

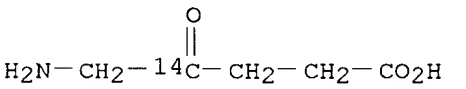
IT **13855-42-0P 13855-43-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 13855-42-0 CAPLUS
CN Levulinic-1-14C acid, 5-amino- (8CI) (CA INDEX NAME)



RN 13855-43-1 CAPLUS
CN Glutaric-1,5-14C2 acid, 3-glycyl-, hydrochloride (8CI) (CA INDEX NAME)



L16 ANSWER 45 OF 45 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1967:54979 CAPLUS
DOCUMENT NUMBER: 66:54979
TITLE: New methods of synthesis of carbon-14 and tritium-labeled .delta.-aminolevulinic acid. I. .delta.-Aminolevulinic-4-14C acid with allylacetic-1-14C and as intermediate
AUTHOR(S): Pichat, Louis; Loheac, Joel; Herbert, Michel
CORPORATE SOURCE: Serv. Mol. Marquees C.E.N., Saclay, Fr.
SOURCE: Bull. Soc. Chim. Fr. (1966), (10), 3268-70
CODEN: BSCFAS
DOCUMENT TYPE: Journal
LANGUAGE: French
GI For diagram(s), see printed CA Issue.
AB Carbonation of the Mg deriv. of 1-bromo-3-butene with 14CO2 (from Ba14CO3) gave 90% allylacetic-1-14C acid as the K salt. The salt was evapd. and dried at 50.degree. in vacuo (Hg vapor). Oxalyl chloride was distd. in and the mixt. left overnight, and then distd. into an Et2O soln. of CH2N2 cooled with liquid N. After 2 hrs. at room temp., HCl was transferred to the mixt. to give 1-chloro-5-hexen-2-one-2-14C which with K phthalide in dimethyl-formamide gave 50% (based on Ba14CO3) 1-phthalimido-5-hexen-2-one-2-14C (I), m. 70.degree.. Ozonolysis gave .delta.-phthalimidolevulinic-4-14C acid which on acid hydrolysis gave crude .delta.-aminolevulinic-4-14C acid. This was purified by chromatography on Dowex 50W-12. The overall yield was 30% and the specific activity was 3 mc./millimole.
IT **7729-71-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 7729-71-7 CAPLUS
CN Pentanoic-4-14C acid, 5-amino-4-oxo- (9CI) (CA INDEX NAME)



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Searched by Barb O'Bryen, STIC 308-4291

substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

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L17  ANSWER 1 OF 4  CAOLD  COPYRIGHT 2001 ACS
ACCESSION NUMBER:  CA62:13034e  CAOLD
TITLE:             synthesis of 5-aminolevulinic-5-14C acid and
                   4,5-dioxovaleric-5-14C acid
AUTHOR NAME:       Gnuchev, N. V.; Neiman, L. A.; Poznanskaya, A. A.
INDEX TERM:        1114-86-9   1187-95-7   2781-46-6   2781-47-7
                   3055-20-7
IT   2781-47-7
RN   2781-47-7  CAOLD
CN   Pentanoic-5-14C acid, 5-amino-4-oxo-, hydrochloride (9CI)  (CA INDEX NAME)
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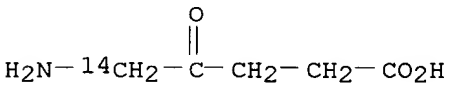

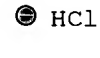

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L17  ANSWER 2 OF 4  CAOLD  COPYRIGHT 2001 ACS
ACCESSION NUMBER:  CA52:256b  CAOLD
TITLE:             synthesis of isotope tagged .delta.-aminolevulinic acid-HCl
                   - (II) .delta.-aminolevulinic acid-4-C14-HCl
AUTHOR NAME:       Pichat, Louis; Herbert, M.
     PATENT NO.    KIND         DATE
     ------------  -----------  ----
PI   GB 778423
INDEX TERM:        16387-80-7 114985-46-5 120087-04-9
IT  16387-80-7
RN   16387-80-7  CAOLD
CN   Pentanoic-4-14C acid, 5-amino-4-oxo-, hydrochloride (9CI)  (CA INDEX NAME)
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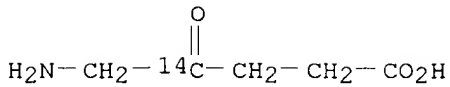
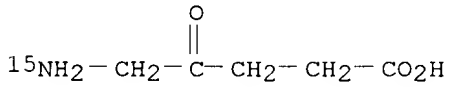
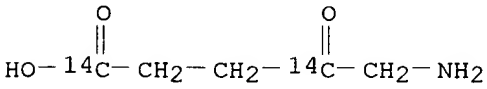


L17 ANSWER 3 OF 4 CAOLD COPYRIGHT 2001 ACS
ACCESSION NUMBER: CA51:7360f CAOLD
TITLE: synthesis of .delta.-aminolevulinic acid-HCl labeled with N15
AUTHOR NAME: Pichat, Louis; Hucleux, M.; Herbert, M.
INDEX TERM: 53856-93-2 109311-38-8 110357-63-6 **116571-80-3**
IT **116571-80-3**
RN 116571-80-3 CAOLD
CN Pentanoic acid, 5-(amino-15N)-4-oxo-, hydrochloride (9CI) (CA INDEX NAME)



L17 ANSWER 4 OF 4 CAOLD COPYRIGHT 2001 ACS
ACCESSION NUMBER: CA51:544e CAOLD
TITLE: biosynthesis of the porphyrinlike moiety of vitamin B12
AUTHOR NAME: Shemin, David; Corcoran, J. W.; Rosenblum, C.; Miller, I. M.
INDEX TERM: **116571-81-4**
IT **116571-81-4**
RN 116571-81-4 CAOLD
CN Levulinic-1,4-14C2 acid, 5-amino- (6CI) (CA INDEX NAME)



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FILE COVERS 1971 TO PATENT PUBLICATION DATE: 16 Jan 2001 (20010116/PD)
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HIGHEST PATENT NUMBER: US6175957
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REVISED CLASS FIELDS (/NCL) LAST RELOADED: Sep 2000
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Sep 2000
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L3              STR
L4              SCR 2039
L6              SCR 2045 OR 2046
L8           35 SEA FILE=REGISTRY SSS FUL L3 AND L4 NOT L6
L11             STR
L12             STR
L13             STR
L15          29 SEA FILE=REGISTRY SUB=L8 SSS FUL (L3 NOT ((L11 OR L12 OR
                L13)))
L18           0 SEA FILE=USPATFULL ABB=ON  L15
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